Kramers Equation and Supersymmetry

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Hamilton's equations with noise and friction possess a hidden supersymmetry, valid for time-independent as well as periodically time-dependent systems. It is used to derive topological properties of critical points and periodic trajectories in an elementary way. From a more practical point of view, the formalism provides new tools to study the reaction paths in systems with separated time scales. A 'reduced current' which contains the relevant part of the phase space probability current is introduced, together with strategies for its computation.

1. INTRODUCTION

Morse theory describes the relationship between the critical points of a smooth real ('Morse') function and the topology of the manifold on which it is defined[1]. It is a major tool in mathematics, but also finds natural applications in physics, for instance in the classification of periodic orbits in classical mechanics.

An elementary and elegant derivation of Morse theory was obtained years ago[2] through the use of supersymmetric quantum mechanics (SUSY-QM), in which the potential is related to the Morse function. It is based on the fact that the semi-classical lowest eigenstates of the SUSY-QM Hamiltonian are concentrated on the saddle-points of the function—those having k fermions on saddles with k unstable directions. The supersymmetry operators that map eigenstates with k fermions into eigenstates with $k \pm 1$ fermions then induce relations between the corresponding saddles.

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Soon after this development, it became clear that the SUSY-QM Hamiltonian—or, more precisely, its zero-fermion restriction—is related by a change of basis to the (Fokker-Planck) equation describing the evolution of probability associated with a Langevin process[3−6], the semi-classical limit now becoming the low temperature limit. In this basis the lowest eigenstates with k fermions are concentrated, rather than on saddle points with k unstable directions, on the unstable manifolds emanating from them. For example, one-fermion eigenvectors with small eigenvalues are peaked on the gradient paths joining two minima via a saddle point, and so represent the reaction current.[7]

A low-temperature Langevin process is a practical method to locate minima of the potential: the dynamics consist of gradient descents, and the small noise allows to escape local minima - a form of what is known as 'simulated annealing'. In the language of SUSY-QM, such a process corresponds to the evolution in zero-fermion subspace. One is then led to ask whether a dynamics associated with the one-fermion subspace can give a 'simulated annealing' scheme that will converge to reaction paths, just as the ordinary one does for metastable states. Indeed, this is so,[7,8] and has been proposed as a basis for numerical algorithms.

In practical applications it is sometimes necessary to extend the overdamped Langevin treatment to a case where inertia plays a role. This is possible because pure Hamilton's equations have themselves a supersymmetry, whose consequences have been explored extensively by Gozzi, Niemi and their co-workers.[9−14] There is however a problem that makes the formalism less transparent than in the Langevin case: in classical mechanics the (Liouville) equations for the evolution of probability in phase-space do not contain second derivatives: the spectrum of the evolution operator is then continuous and the space of wavefunctions awkward. A natural cure to this problem, both from the analytical and the practical point of view, is the introduction of noise and friction so that we study a more general process:

$$
\begin{cases}
\dot{q}_i = p_i \\
\dot{p}_i = -\dfrac{\partial V}{\partial q_i} - \gamma p_i + \sqrt{2\gamma T}\,\eta_i,
\end{cases}
\tag{1}
$$

$V(\boldsymbol{q})$ is a potential energy, η_i are Gaussian white noises modelling the interaction with a thermal bath at temperature T, while γ is the coupling to the bath (physically a friction coefficient). The dynamics (1) can be expressed as a probability density evolving according to the Kramers equation[15]:

$$
\frac{\partial P(\mathbf{q}, \mathbf{p}, t)}{\partial t} = \left[\sum_{i=1}^{N} \frac{\partial}{\partial p_i} \left(\gamma T \frac{\partial}{\partial p_i} + \gamma p_i + \frac{\partial V}{\partial q_i} \right) - \frac{\partial}{\partial q_i} p_i \right] P(\mathbf{q}, \mathbf{p}, t)
$$

$$
= -H_K P(\mathbf{q}, \mathbf{p}, t).
\tag{2}
$$

It turns out that one can uncover a hidden supersymmetry associated with this equation, just as there is SUSY-QM associated with the Fokker-Planck equation

without inertia. As we shall see, this leads to a non-Hermitian supersymmetric quantum mechanics, whose zero-fermion restriction is the Kramers equation. The higher fermion-number subspaces contain, again just as in SUSY-QM, the information on the fixed points and their stable and unstable manifolds, where stability is now defined with respect to Hamiltonian dynamics perturbed by friction. Perhaps more surprising is the fact that one can generalize these results to the case in which the Hamiltonian depends periodically on time—one then has a supersymmetric structure in the Floquet representation. This supersymmetry has a series of consequences which we shall also explore.

The organization of this paper is as follows: in Section 2 we construct the extension of the Kramers operator and we discuss the consequences its supersymmetry has on the organization of the eigenvectors and eigenvalues. In Section 3 we study the low-temperature ('semi-classical') limit using standard path-integral methods, and show that it is dominated by periodic trajectories—in particular fixed points—of the noiseless dynamics. In Section 4 we use these results to show how one can rederive Morse theory results using time-independent Hamiltonians. As an alternative, a WKB treatment of the time-independent case with conservative forces is possible (Section 5): it does not rely on path integrals and is very close to the treatment of SUSY-QM, with the only complication of non-Hermiticity. In Section 6 we present the supersymmetries associated with a periodically time-dependent Hamiltonian, and give a first few applications.

Just as the zero fermion subspace corresponds to Kramers' equation, and this in turn to a process following Hamilton's equations plus noise and friction, one may ask to what stochastic processes does the $k > 0$ fermion subspaces correspond. In Section 7 we devise such processes, and use them to give a constructive (and quite non-rigorous) derivation of the low-temperature wavefunctions yielding the Morse complex. As mentioned above, part of the motivation for this work is the construction of algorithms to find saddle points and reaction paths between metastable states, a very important problem in Physical Chemistry. In Section 8 we show the relation between one-fermion wavefunctions and reaction currents. Interestingly enough, the formalism strongly suggests that rather than studying the currents themselves, a modified 'reduced current' should be used, which contains only the part of the current that is effective in making transitions, equilibrium circulations within states being subtracted. Finally, in the Conclusion we outline the several possible continuations of this work.

2. SUSY OF KRAMERS DYNAMICS

2.1. The Hamiltonian Case

The Hamiltonian dynamics

$$\dot{q}_i = \frac{\partial \mathcal{H}}{\partial p_i}; \qquad \dot{p}_i = -\frac{\partial \mathcal{H}}{\partial q_i}, \tag{3}$$

where $\mathcal{H}$ is the Hamiltonian function, induces an evolution for probabilities $P(\mathbf{q}, \mathbf{p})$ in phase-space given by

$$\frac{\partial P}{\partial t} = -H_{\mathcal{H}}P, \quad \text{with} \quad H_{\mathcal{H}} = -\sum_{i=1}^{N}\left(\frac{\partial \mathcal{H}}{\partial q_i}\frac{\partial}{\partial p_i} - \frac{\partial \mathcal{H}}{\partial p_i}\frac{\partial}{\partial q_i}\right). \tag{4}$$

One can uncover a group of symmetries of $H_{\mathcal{H}}$ by extending the space with $4N$ fermion operators $(a_i, a_i^\dagger, b_i, b_i^\dagger)$, and writing[9–11]:

$$H_{\mathcal{H}}^S = -\sum_{i=1}^{N}\left(\frac{\partial \mathcal{H}}{\partial q_i}\frac{\partial}{\partial p_i} - \frac{\partial \mathcal{H}}{\partial p_i}\frac{\partial}{\partial q_i}\right) + \frac{\partial^2 \mathcal{H}}{\partial q_i \partial q_j}b_i^\dagger a_j - \frac{\partial^2 \mathcal{H}}{\partial p_i \partial p_j}a_j^\dagger b_i$$

$$+ \frac{\partial^2 \mathcal{H}}{\partial p_j \partial q_i}(b_i^\dagger b_j - a_j^\dagger a_i), \tag{5}$$

which reduces to the original $H_{\mathcal{H}}$ in the zero-fermion subspace. $H_{\mathcal{H}}^S$ has a large group of symmetries, generated by the operator whose action is to multiply by $\mathcal{H}$ (and other constants of motion, if present), and by

$$K = \sum_{i=1}^{N} a_i b_i; \qquad K^\dagger = -\sum_{i=1}^{N} a_i^\dagger b_i^\dagger; \qquad F = \sum_{i=1}^{N}(a_i^\dagger a_i + b_i^\dagger b_i)$$

$$Q_1 = -i\sum_{i=1}^{N}\left(\frac{\partial}{\partial q_i}a_i + \frac{\partial}{\partial p_i}b_i\right);$$

$$Q_2 = [K^\dagger, Q_1]_- = -i\sum_{i=1}^{N}\left(\frac{\partial}{\partial q_i}b_i^\dagger - \frac{\partial}{\partial p_i}a_i^\dagger\right) \tag{6}$$

$$Q_3 = [Q_2, \mathcal{H}]_- = -i\sum_{i=1}^{N}\left(\frac{\partial \mathcal{H}}{\partial q_i}b_i^\dagger - \frac{\partial \mathcal{H}}{\partial p_i}a_i^\dagger\right);$$

$$Q_4 = [Q_1, \mathcal{H}]_- = -i\sum_{i=1}^{N}\left(\frac{\partial \mathcal{H}}{\partial q_i}a_i + \frac{\partial \mathcal{H}}{\partial p_i}b_i\right).$$

The supersymmetric charges are nilpotent:

$$Q_1^2 = Q_2^2 = Q_3^2 = Q_4^2 = 0, \tag{7}$$

and

$$H_{\mathcal{H}}^S = (Q_1 + Q_2 + Q_3)^2. \tag{8}$$

As already mentioned in the Introduction, the question of the spectra of operators and the underlying Hilbert space is rather tricky, because all operators have at most

first order derivatives. Here we shall work with the Kramers equation, for which all relevant operators have discrete spectra, the Hilbert space is tractable, but the symmetry group is considerably smaller.

2.2. Extended Operator and Symmetries

Let us go back to the original Kramers dynamics with inertia and dissipation (1), which we shall write in a more general form[3]:

$$
\begin{cases}
\dot{q}_i = \dfrac{\partial \mathcal{H}}{\partial p_i} \\[2mm]
\dot{p}_i = -\dfrac{\partial \mathcal{H}}{\partial q_i} - \gamma \dfrac{\partial \mathcal{H}}{\partial p_i} + \sqrt{2\gamma T}\,\eta_i.
\end{cases}
\tag{9}
$$

Here $\mathcal{H}$ is a general Hamiltonian function of $\{\mathbf{q}, \mathbf{p}\}$ coordinates, Eq. (1) corresponds to $\mathcal{H}$ of the particular form $\mathcal{H} = \mathbf{p}^2/2 + V(\mathbf{q})$. We shall hence assume that $\mathcal{H}$ is a smooth function, either defined over a bounded phase-space $\{\mathbf{q}, \mathbf{p}\}$ or growing fast enough at infinity. The probability density in the phase space evolves as:

$$
\frac{\partial P(\mathbf{q}, \mathbf{p}, t)}{\partial t} = - H_K P(\mathbf{q}, \mathbf{p}, t).
$$

$$
\text{with} \quad H_K = -\gamma \sum_{i=1}^{N} \frac{\partial}{\partial p_i}\left(T \frac{\partial}{\partial p_i} + \frac{\partial \mathcal{H}}{\partial p_i}\right) - \sum_{i=1}^{N}\left(\frac{\partial \mathcal{H}}{\partial q_i}\frac{\partial}{\partial p_i} - \frac{\partial \mathcal{H}}{\partial p_i}\frac{\partial}{\partial q_i}\right)
\tag{10}
$$

One can easily see that the Gibbs density $(e^{-\frac{\mathcal{H}}{T}})$ is the stationary state of the process, the eigenstate of H_K with zero eigenvalue.

In order to construct a fermionic extension we start from the observation that the previous symmetry charge Q_1 is independent of the dynamics considered, having only a geometrical meaning (it is related to the so-called exterior derivative). We then propose

$$
Q = Q_1 = -i \sum_{i=1}^{N}\left(\frac{\partial}{\partial q_i} a_i + \frac{\partial}{\partial p_i} b_i\right),
\tag{11}
$$

---

[3] for a discussion on the different possibilities to connect a classical evolution with a thermal bath see[19]

as one of the supersymmetric charges. By inspection, one can see that

$$
\begin{aligned}
H = H_K + \sum_{i,j} \Bigg(& \frac{\partial^2 \mathcal{H}}{\partial q_i \partial q_j} b_i^\dagger a_j + \gamma \frac{\partial^2 \mathcal{H}}{\partial p_i \partial p_j} b_j^\dagger b_i - \frac{\partial^2 \mathcal{H}}{\partial p_i \partial p_j} a_i^\dagger b_j \\
& + \frac{\partial^2 \mathcal{H}}{\partial q_i \partial p_j} (\gamma b_j^\dagger a_i + b_i^\dagger b_j - a_j^\dagger a_i) \Bigg)
\end{aligned}
\tag{12}
$$

has Q as a symmetry. By analogy with the Hamiltonian case one may ask if there is a first order differential operator $\bar{Q}$ satisfying:

$$
\bar{Q}^2 = Q^2 = 0, \quad T[Q, \bar{Q}]_+ = T(Q + \bar{Q})^2 = H.
\tag{13}
$$

This is so with:

$$
\bar{Q} = -i \sum_{i=1}^N \left[b_i^\dagger \left(\frac{\partial}{\partial q_i} + \frac{1}{T} \frac{\partial \mathcal{H}}{\partial q_i} \right) - a_i^\dagger \left(\frac{\partial}{\partial p_i} + \frac{1}{T} \frac{\partial \mathcal{H}}{\partial p_i} \right) + \gamma b_i^\dagger \left(\frac{\partial}{\partial p_i} + \frac{1}{T} \frac{\partial \mathcal{H}}{\partial p_i} \right) \right].
\tag{14}
$$

Thus, we now have a supersymmetric extension of H_K and the corresponding charges[4]. The large algebra of symmetries (6) of the classical formalism has become much smaller; just as in the case of SUSY-QM, only Q, $\bar{Q}$ and F are symmetries.

The system (9) can be written in terms of the variables $(x_1, \ldots, x_{2N}) = (\boldsymbol{q}, \boldsymbol{p})$ in a more compact way as:

$$
\dot{x}_i = -\sum_j \Omega_{ij} \frac{\partial \mathcal{H}}{\partial x_j} + D_{ij} \left(\frac{\partial \mathcal{H}}{\partial x_j} - \sqrt{\frac{2T}{\gamma}} \eta_j \right) \quad \Omega_{ij} = \begin{pmatrix} 0_N & -1_N \\ 1_N & 0_N \end{pmatrix} \quad D_{ij} = \gamma \begin{pmatrix} 0 & 0 \\ 0 & 1_N \end{pmatrix}.
\tag{15}
$$

When $D_{ij} = 0$, (15) is the usual simplectic formulation of Hamilton's equation, the second term of the r.h.s represents the interaction with the bath. With this notation, the generalized Fokker-Planck Hamiltonian (12) becomes:

$$
\begin{aligned}
H &= -\sum_{i,j} \frac{\partial}{\partial x_i} \left(D_{ij} \left(T \frac{\partial}{\partial x_j} + \frac{\partial \mathcal{H}}{\partial x_j} \right) + \Omega_{ij} \frac{\partial \mathcal{H}}{\partial x_j} \right) + \sum_{i,j,k} (D_{ij} + \Omega_{ij}) \frac{\partial^2 \mathcal{H}}{\partial x_k \partial x_j} c_i^\dagger c_k, \\
&= H_K + \sum_{i,k} A_{ik} c_i^\dagger c_k,
\end{aligned}
\tag{16}
$$

where $(c_1, \ldots, c_{2N}) = (a_1, \ldots, a_N, b_1, \ldots, b_N)$, and we have defined:

$$
A_{ik} = \sum_j (D_{ij} + \Omega_{ij}) \frac{\partial^2 \mathcal{H}}{\partial x_k \partial x_j}.
\tag{17}
$$

---

[4] These symmetries have already been obtained by Kleinert and co workers,[20] for an action corresponding to an evolution of the form (1) in the (Lagrangian) path-integral formalism.

The charges are:

$$
\begin{cases}
Q = -i \sum_{i=1}^{2N} \frac{\partial}{\partial x_i} c_i \\
\bar{Q} = -\frac{i}{T} \sum_{i=1}^{2N} (\Omega_{ij} + D_{ij}) \left(T \frac{\partial}{\partial x_j} + \frac{\partial \mathcal{H}}{\partial x_j} \right) c_i^\dagger = e^{-\beta \mathcal{H}} (-i) \sum_{i=1}^{2N} (\Omega_{ij} + D_{ij}) \frac{\partial}{\partial x_j} c_i^\dagger \, e^{\beta \mathcal{H}}.
\end{cases}
$$
(18)

The notation in this section has been specialized to the case in which all the phase space velocities derive from a global function $\mathcal{H}$. Let us keep in mind, however, that when this is not the case, and the dynamics is given by:

$$
\dot{x}_i = -\sum_j (\Omega_{ij} \mathcal{H}_j + D_{ij} \mathcal{H}_j) - \sqrt{\frac{2T}{\gamma}} \eta_i,
$$
(19)

with $\frac{\partial \mathcal{H}_i}{\partial x_j} = \frac{\partial \mathcal{H}_j}{\partial x_i}$ but $\mathcal{H}_j(x)$ not globally a gradient, there still is a supersymmetry:

$$
Q = -i \sum_{i=1}^{2N} \frac{\partial}{\partial x_i} c_i \qquad \bar{Q} = -\frac{i}{T} \sum_{i=1}^{2N} A_{ik} \left(T \frac{\partial}{\partial x_j} + \mathcal{H}_j \right) c_i^\dagger
$$

$$
H = -\sum_{i,j} \frac{\partial}{\partial x_i} \left(D_{ij} \left(T \frac{\partial}{\partial x_j} + \mathcal{H}_j \right) + \Omega_{ij} \mathcal{H}_j \right) + \sum_{i,k} A_{ik} c_i^\dagger c_k \quad \text{with} \quad (20)
$$

$$
A_{ik} = \sum_j (D_{ij} + \Omega_{ij}) \frac{\partial \mathcal{H}_j}{\partial x_k}.
$$

2.3. The Spectrum of H

We shall first examine the case of a time-independent Hamiltonian $\mathcal{H}$, including cases like (20) where there is no global potential. Section 6 will be devoted to the time-dependent case while Sections 4 and 5 will be specifically dedicated to the conservative case with a global $\mathcal{H}$.

H is not hermitian, and cannot be taken to a Hermitian form via a similarity transformation. It acts on functions of the form

$$
|\psi\rangle = \sum \psi_{i_1,\ldots,i_m,j_1,\ldots,j_n}(\mathbf{q}, \mathbf{p}) b_{i_1}^\dagger \ldots b_{i_m}^\dagger a_{j_1}^\dagger \ldots a_{j_n}^\dagger |-\rangle,
$$
(21)

where $|-\rangle$ is the Fermion vacuum. We have to distinguish right and left eigenvectors. They are defined as:

$$
H |\psi_i^R\rangle = \lambda_i |\psi_i^R\rangle \quad \text{and} \quad H^\dagger |\psi_i^L\rangle = \lambda_i^* |\psi_i^L\rangle.
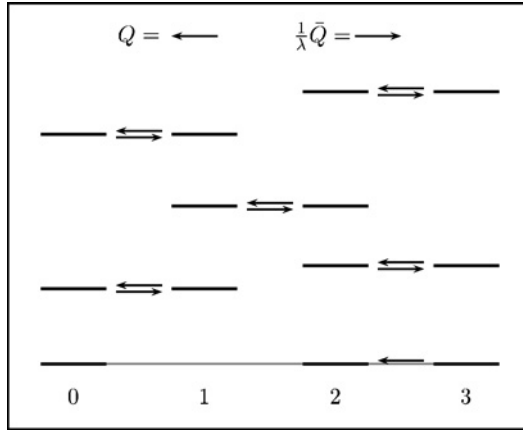$$
(22)

Fig. 1. Generic representation of the spectrum of H. The eigenstates are divided in two kinds: pairs of eigenstates made via Q and unpaired eigenstates, which does not belong to any pair by Q. The latter are only present in the $\lambda = 0$ eigenspace.

In what follows we shall suppose that H is diagonalizable i.e. one can find a bi-orthonormal eigenbasis[5]:

$$\langle \psi_j^L | \psi_i^R \rangle = \delta_{\lambda_i, \lambda_j}. \tag{23}$$

The purpose of the two following subsections is to show that the organization of the spectrum is as in Fig. 1.

2.3.1. Eigenvectors with Non-zero Eigenvalues

Eigenvectors with $\lambda \neq 0$ are not annihilated by both Q and $\bar{Q}$. As Q and $\bar{Q}$ commute with H, they map eigenvectors into eigenvectors with the same eigenvalue. This yields for the $\lambda \neq 0$ spectrum a structure of degenerate pairs connected by Q and $\bar{Q}$. One can indeed construct a basis $(|\phi_i^R\rangle, |\chi_i^R\rangle)$ such that:

$$Q|\phi_i^R\rangle = |\chi_i^R\rangle \quad \text{and} \quad \bar{Q}|\chi_i^R\rangle = \frac{\lambda_i}{T}|\phi_i^R\rangle. \tag{24}$$

To see this, first notice that a general eigenstate $|\psi^R\rangle$ of eigenvalue $\lambda \neq 0$ is the sum of two eigenstates $|\phi^R\rangle$ and $|\chi^R\rangle$ annihilated by $Q\bar{Q}$ and $\bar{Q}Q$ respectively. Indeed, denoting $|\chi^R\rangle \equiv Q\bar{Q}|\psi^R\rangle$ and $|\phi^R\rangle \equiv \bar{Q}Q|\psi^R\rangle$ we have:

$$|\psi^R\rangle = \frac{1}{\lambda}H|\psi^R\rangle = \frac{T}{\lambda}(|\chi^R\rangle + |\phi^R\rangle). \tag{25}$$

---

[5] Diagonalizability is not entirely obvious even in the pure Kramers (zero-fermion) case, see [21] for a discussion.

Using the fact that $Q\bar{Q}$ and $\bar{Q}Q$ both commute with H, $|\chi^R\rangle$ and $|\phi^R\rangle$ are also eigenvectors of H with eigenvalue λ, and are annihilated respectively by $\bar{Q}Q$ and $Q\bar{Q}$. One thus constructs a basis of the whole eigenspace $\lambda \neq 0$ as the union of bases of eigenvectors annihilated by $\bar{Q}Q$ on one hand, and $Q\bar{Q}$ on the other hand. We do this as follows: denote $|\chi_i^R\rangle$ a basis of eigenvectors annihilated by $\bar{Q}Q$, and define $|\phi_i^R\rangle \equiv \frac{T}{\lambda_i}\bar{Q}|\chi_i^R\rangle$. Because $Q|\phi_i^R\rangle = \frac{1}{\lambda_i}H|\chi_i^R\rangle = |\chi_i^R\rangle$, the $|\phi_i^R\rangle$ so defined are independent, since one can map them back into an independent set with Q.

Furthermore, the $|\phi_i^R\rangle$ generate all the eigenvectors with $\lambda \neq 0$ annihilated by $Q\bar{Q}$. Indeed, take one such $|\psi^R\rangle$. One clearly has $|\psi^R\rangle = \frac{T}{\lambda}\bar{Q}Q|\psi^R\rangle$. As $Q|\psi^R\rangle$ is annihilated by $\bar{Q}Q$, it can be developed as $Q|\psi^R\rangle = \sum_i \alpha_i|\chi_i^R\rangle$, and hence $|\psi^R\rangle = \frac{T}{\lambda}\sum_i \alpha_i\bar{Q}|\chi_i^R\rangle = \frac{1}{\lambda}\sum_i \alpha_i\lambda_i|\phi_i^R\rangle$.

The family $(|\phi_i^R\rangle, |\chi_i^R\rangle)$ is thus a basis of the whole $\lambda_i \neq 0$ spectrum, which satisfy the pairing property (24). As to the left eigenvectors, the structure is the same. Constructing a basis with

$$\langle\phi_i^L\phi_j^R\rangle = \delta_{ij} \qquad \langle\chi_i^L\chi_j^R\rangle = \delta_{ij}$$
$$\langle\phi_i^L\chi_j^R\rangle = 0 \qquad \langle\chi_i^L\phi_j^R\rangle = 0, \tag{26}$$

the left eigenvectors are paired according to:

$$Q^\dagger|\chi_i^L\rangle = |\phi_i^L\rangle \qquad \bar{Q}^\dagger|\phi_i^L\rangle = \frac{\lambda_i^*}{T}|\chi_i^L\rangle. \tag{27}$$

2.3.2. Zero Eigenvalues and Topology

The scenario in the $\lambda = 0$ eigenspace is a little more complex. Let us argue that one can in principle build a basis of right eigenvectors (we drop the index R within this subsection) composed of (see Fig. 1):

i) pairs $(|\phi_i^{k+1}\rangle, |\chi_i^k\rangle)$ such that $|\chi_i^k\rangle = Q|\phi_i^{k+1}\rangle \neq 0$

ii) unpaired eigenstates $|\rho_i^k\rangle$ such that $Q|\rho_i^k\rangle = 0$ and $\forall|\psi\rangle\ |\rho_i^k\rangle \neq Q|\psi\rangle$, (28)

where k denotes the number of Fermions. Note that such a basis is matched by the corresponding one for the left eigenvectors.

We shall now construct a basis satisfying (28). Let us first look at the 0 fermion sector. All the eigenvectors are annihilated by the a_i and consequently by Q. Some of them are the image by Q of other eigenvectors, and some are not. Let us note $|\chi_i^0\rangle$ a basis of the former, and $|\phi_i^1\rangle$ the 1-fermion eigenvectors which generate them: $|\chi_i^0\rangle = Q|\phi_i^1\rangle$. The $|\chi_i^0\rangle$ may not be a basis of the zero fermion sector and one can complete them with eigenvectors $|\rho_i^0\rangle$. By definition, the $|\rho_i^0\rangle$ are annihilated by Q but are not the image of any other eigenvectors by Q. At this point, $\{|\chi_i^0\rangle, |\rho_i^0\rangle\}$ constitutes a basis of the 0 fermion sector satisfying (28). One

can then turn to the 1 fermion sector. The part of this sector which is annihilated by Q can be organized as the 0 fermion number, that is there exist a basis $\{|\chi_i^1\rangle, |\rho_i^1\rangle\}$ which generates this part, and eigenvectors $|\phi_i^2\rangle$ such that $|\chi_i^1\rangle = Q|\phi_i^2\rangle$. The family $|\phi_i^1\rangle$ introduced above completes the $\{|\chi_i^1\rangle, |\phi_i^1\rangle\}$ in a basis of the whole 1 fermion sector. This construction can be followed for every fermion sector and allows us to construct inductively a basis $\{|\chi_i^k\rangle, |\phi_i^k\rangle, |\rho_i^k\rangle\}$ which satisfy (28).

In the usual SUSY-QM, only unpaired states exist in the zero eigenvalue subspace. Indeed, we shall show in Section 5 that this is also the case for a Kramers problem with time-independent forces that derive from a global potential. Note however, that states paired by $\bar{Q}$ with $\lambda = 0$ can exist: a system living on a ring encircling a magnetic flux has no global potential and there is a pair by $\bar{Q}$.

The eigenstates $|\rho_i^k\rangle$ are related to the topology of the phase-space because $Q^\dagger$ is the exterior derivative acting on (left) states with k fermions (the differential k-forms). They span a space whose dimension is the kth Betti number B_k, and is isomorphic to the so-called k^{th} de Rham cohomology group[16] associated with the phase space.

The basis of the $\lambda = 0$ and $\lambda \neq 0$ eigenspaces form a global basis: $\{|\psi_i\rangle\} \equiv \{|\chi_i^R\rangle, |\phi_i^R\rangle, |\rho_i^R\rangle\}$. Given its structure, it is tempting to denote the states generated by $\{|\rho_i^R\rangle\}$ and $\{|\phi_i^R\rangle, |\chi_i^R\rangle\}$ as "unpaired" and "paired", respectively, even if one can construct states which are not paired by Q without being generated by the $|\rho_i^k\rangle$.

3. LOW-TEMPERATURE LIMIT: FIXED POINTS AND PERIODIC ORBITS

3.1. Fixed Points and Periodic Orbits

To study the low-lying eigenvectors in the limit of small T, we shall compute the trace of the evolution operator for different values of t and use the result to reconstruct the spectrum. A quick method to do this is to write a path integral and use saddle point evaluation. This is a standard exercise which we report in Appendix A. When the temperature goes to zero, one finds that the path integral is dominated by the noiseless periodic trajectories which satisfy:

$$\begin{cases} \dot{p}_i^c = -\dfrac{\partial \mathcal{H}}{\partial q_i} - \gamma \dfrac{\partial \mathcal{H}}{\partial p_i} \\[2mm] \dot{q}_i^c = \dfrac{\partial \mathcal{H}}{\partial p_i}. \end{cases} \tag{29}$$

To obtain the next order, one develops the coordinates as a small perturbation $x_i' = (q_i', p_i')$ around each noiseless orbits $x_i^c = (q_i^c, p_i^c)$

$$x_i = x_i^c + \sqrt{T}x_i'. \tag{30}$$

The contribution of each orbit x^c can be seen as the trace of $\mathcal{T}e^{-\int_0^t H^c(t')dt'}$, with:

$$
H^c = \frac{\partial}{\partial q_i'}\left(p_j'\left.\frac{\partial^2\mathcal{H}}{\partial p_i\partial p_j}\right|_{q^c,p^c} + q_j'\left.\frac{\partial^2\mathcal{H}}{\partial p_i\partial q_j}\right|_{q^c,p^c}\right) - \frac{\partial}{\partial p_i'}\left(\gamma T\frac{\partial}{\partial p_i} + \gamma\, p_j'\left.\frac{\partial^2\mathcal{H}}{\partial p_i\partial p_j}\right|_{q^c,p^c}\right.
$$

$$
\left.+\gamma\, q_j'\left.\frac{\partial^2\mathcal{H}}{\partial p_i\partial q_j}\right|_{q^c,p^c} + p_j'\left.\frac{\partial^2\mathcal{H}}{\partial q_i\partial p_j}\right|_{q^c,p^c} + q_j'\left.\frac{\partial^2\mathcal{H}}{\partial q_i\partial q_j}\right|_{q^c,p^c}\right) + \left.\frac{\partial^2\mathcal{H}}{\partial q_i\partial q_j}\right|_{q^c,p^c} b_i^\dagger a_j
$$

$$
+\gamma\left.\frac{\partial^2\mathcal{H}}{\partial p_i\partial p_j}\right|_{q^c,p^c} b_j^\dagger b_i - \left.\frac{\partial^2\mathcal{H}}{\partial p_i\partial p_j}\right|_{q^c,p^c} a_i^\dagger b_j + \left.\frac{\partial^2\mathcal{H}}{\partial p_j\partial q_i}\right|_{q^c,p^c}(\gamma b_j^\dagger a_i + b_i^\dagger b_j - a_j^\dagger a_i)
$$

$$
H^c = -\frac{\partial}{\partial x_k'}\left(D_{kj}\frac{\partial}{\partial x_j'} + A_{kj}^c(t)x_j'\right) + A_{ij}^c(t)c_i^\dagger c_j,
$$

$$(31)$$

where $A_{ij}^c(t)$ is defined as in (17), but evaluated along the classical periodic orbit (which in certain cases will just be a fixed point):

$$
A_{ik}^c(t) \equiv A_{ik}[x^c(t)] = (D_{ij} + \Omega_{ij})\left.\frac{\partial\mathcal{H}}{\partial x_k\partial x_j}\right|_{x^c}. \tag{32}
$$

Here we have adopted a notation involving a global potential $\mathcal{H}$, although this is not necessary: if there is no global $\mathcal{H}$ it suffices to write (31) with A_{kj}^c defined as in (20).

Note that to this order fermionic and bosonic parts are decoupled. Eq. (31) is nothing but the SUSY Hamiltonian corresponding to a diffusion on a time-dependent harmonic potential $\mathcal{H}^c = \frac{1}{2}\frac{\partial^2\mathcal{H}}{\partial x_i\partial x_j}x_i'x_j'$, corresponding to

$$
\dot{x}_i' = -A_{ij}^c(t)x_j' + D_i\eta_i, \tag{33}
$$

where η_i is a Gaussian white noise.

A compact way of expressing the spectral properties of the evolution operator is via the generating function:

$$
T(\lambda,t) \equiv \mathrm{Tr}\left(\lambda^F\mathcal{T}e^{-\int H(t')dt'}\right) = \sum_k \lambda^k\mathrm{Tr}\left(\mathcal{T}e^{-\int H(t')dt'}\right)\big|_{k\text{ ferm.}}, \tag{34}
$$

where $\mathcal{T}$ denotes time order and F is the Fermion number (6). To leading order in the temperature T, we have to compute $T(\lambda,t)$ as a sum over the contributions $T^c(\lambda,t)$ around each periodic orbit:

$$
T(\lambda,t) \sim \sum_k \lambda^k \sum_{\substack{\text{noiseless}\\\text{orbits c}}} \mathrm{Tr}\left(\mathcal{T}e^{-\int H^c(t')dt'}\right)\big|_{k\text{ ferm.}} \equiv \sum_{\substack{\text{noiseless}\\\text{orbits c}}} T^c(\lambda,t). \tag{35}
$$

Because boson and fermion degrees of freedom are decoupled to this order, each term of the sum is a product of a trace over boson and a trace over fermion degrees of freedom—both with a (in general time-dependent) harmonic oscillator.

Again, this is a standard exercise which we do in detail in Appendix B. The result is that for every orbit the boson degrees of freedom contribute with a factor $|\det(1 - U^c(t))|^{-1}$, while the fermion ones with $\det(1 + \lambda U^c(t))$, where $U^c(t)$ is a $2N \times 2N$ matrix defined by:

$$\dot{U}^c(t') = -A^c(t')U^c(t') \qquad\qquad U^c(0) = 1. \tag{36}$$

We have then, to leading order in T:

$$T(\lambda, t) \xrightarrow[T \to 0]{} \sum_{\substack{\text{noiseless} \\ \text{orbits c}}} \frac{\det(1 + \lambda U^c(t))}{|\det(1 - U^c(t))|}. \tag{37}$$

This formula has two limitations, both reflecting important features of the phase-space structure:

- If an eigenvalue of U^c is 1 for some orbits, (37) diverges. This can be accidental, e.g. a critical point that is undergoing a second order phase transition, or, more importantly, a consequence of the fact that the orbit is not isolated but belongs to a continuous family, possibly as a result of a symmetry: the problem becomes one of degenerate Morse theory.[6]
- The saddle point evaluation is legitimate to the extent that $T \to 0$ at fixed t. If we are interested in orbits of period going to infinity as $T \to 0$, we have to bear in mind that the action itself will depend on T, and (37) may be invalid. This problem is not specific to our treatment: the long time periodic orbits are a usual pitfall in semi-classical quantization.

3.2. Spectrum of Low Real Eigenvalues

Let us analyze first the contribution to (37) of an isolated orbit whose period equals the period τ of the Hamiltonian:

$$T^c(\lambda, n\tau) \sim \prod_{i=1}^{2N} \frac{1 + \lambda(u_i)^n}{|1 - (u_i)^n|}. \tag{38}$$

where $(u_1, \ldots, u_{2N})$ are the eigenvalues of $U^c(\tau)$ (for simplicity, we omit the supra-index c labelling the noiseless trajectory). One can read in the factor $(1 + \lambda u_i)$ the contribution of the Fermion vacuum whose eigenvalue is 1 plus λ times the contribution of the one-fermion state, whose eigenvalue is u_i. The bosonic counterpart can be read in $\frac{1}{|1-u_i|}$: we shall expand $\frac{1}{|1-u_i^n|}$ as a geometric serie from which we shall recognize the spectrum.

---

[6] For a time-independent system with non-conservative forces for example: a single periodic (non-constant) trajectory is in fact a continuous family of trajectories, each one being the same orbit with a different starting point.

First consider the case of a real u_i. If $|u_i| < 1$, then

$$\frac{1}{|1 - u_i^n|} = \frac{1}{1 - u_i^n} = \sum_{k=0}^{\infty} u_i^{nk}, \tag{39}$$

If $|u_i| > 1$, one can rewrite $|1 - u_i|$ as $|u_i|(1 - \frac{1}{u_i})$. The same development gives:

$$\frac{1}{|1 - u_i^n|} = \text{sign}(u_i) \sum_{k=1}^{\infty} u_i^{-kn}, \quad \forall k \geq 1. \tag{40}$$

Next, consider the case of a pair of complex eigenvalues (u_i, u_i^*). If $|u_i| < 1$ we may write:

$$\frac{1}{|1 - u_i^n|} \frac{1}{|1 - u_i^{*n}|} = \frac{1}{(1 - u_i^n)} \frac{1}{(1 - u_i^{*n})} = \sum_{k=0,k'=0} (u_i)^{nk} (u_i^*)^{nk'}, \tag{41}$$

while, if $|u_i| > 1$:

$$\frac{1}{|1 - u_i^n|} \frac{1}{|1 - u_i^{*n}|} = \sum_{k=1,k'=1} (u_i)^{-nk} (u_i^*)^{-nk'}. \tag{42}$$

All in all, the contribution of the orbit to the spectrum is the tensor product of the following sets (see Fig. 2):
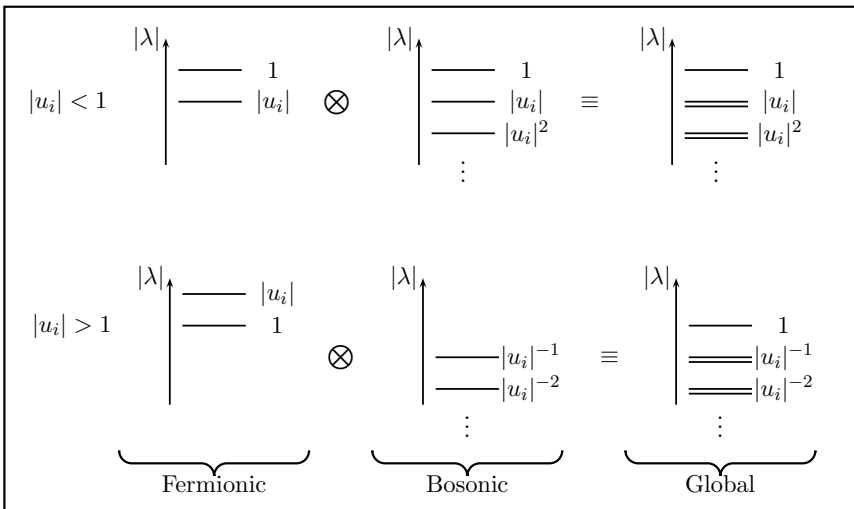

Fig. 2. Structure of the spectrum for $|u_i| < 1$ or $|u_i| > 1$ at leading order in T. The global contribution of the orbit is the tensor product of the bosonic and the fermionic parts. There is a gap of order one in modulus between the most stable state and the first excited one when T goes to zero.

- $(1, u_i) \otimes (1, u_i, u_i^2, \ldots)$ for $u_i = u_i^*$, $|u_i| < 1$;
- $(1, u_i) \otimes (\frac{1}{u_i}, \frac{1}{u_i^2}, \ldots)$ for $u_i = u_i^*$, $|u_i| > 1$;
- $(1, u_i) \otimes (1, u_i, u_i^2, \ldots) \otimes (1, u_i^*) \otimes (1, u_i^*, u_i^{*2}, \ldots)$ for $u_i \neq u_i^*$, $|u_i| < 1$;
- $(1, u_i) \otimes (\frac{1}{u_i}, \frac{1}{u_i^2}, \ldots) \otimes (1, u_i^*) \otimes (\frac{1}{u_i^*}, \frac{1}{u_i^{*2}}, \ldots)$ for $u_i \neq u_i^*$, $|u_i| > 1$.

We have supposed here that the number of real eigenvalues $u_i < -1$ is even.

Let us now consider the contribution of an orbit of primitive period $p\tau$. Clearly, one can start from p different points along the orbit. For each starting point the preceding discussion holds, and one gets for the evolution over time $p\tau$ a spectrum as above, but each level is now p-fold degenerate (to this order in T). The path integral tells us that the contribution of this orbit to any trace over n cycles is zero if n is not a multiple of p, and is p times the contribution of a single starting point otherwise. This can be understood if each multiplet yields, for the evolution over a single period of the Hamiltonian, eigenvalues corresponding to the p different p^{th} roots of those for p cycles—because the sum of the p different roots to the power n is non-zero only if p divides n.

Let us stress that breakdown of (37), for example because one of the $|u_i| = 1$, signals the fact that the spectrum is no longer a superposition of harmonic spectra of frequencies of order one, and that the gap between ground and first excited state will go to zero with T. In such cases, the contribution of the u_i such that $|u_i| \neq 1$ is as described here, and the degrees of freedom in the directions corresponding to $|u_j| = 1$ have to be treated with other methods (collective coordinates, for example).

The main point of this section is that each orbit is associated with one and only one eigenstate of the evolution operator with unit eigenvalue to this order. This eigenstate has k fermions if $U^c(\tau)$ has k eigenvalues with modulus larger than 1: that is to say if its Morse index is k.

4. TIME-INDEPENDENT HAMILTONIAN: A NON-HERMITIAN SUSY QUANTUM MECHANICS AND MORSE THEORY

In the case of a time-independent Hamiltonian deriving from a global potential, we recover the Morse inequalities for the stationary points of the dynamics, by going to the small temperature limit. The geometric structures involved now correspond to the manifolds that are stable and unstable with respect to Hamiltonian dynamics plus friction, instead of simple gradient descents.

If $\mathcal{H}$ is time-independent and conservative, in the presence of non-zero friction, the only periodic orbits that matter are fixed points, as one can see using

(29):

$$\frac{d\mathcal{H}}{dt} = \sum_i \frac{\partial \mathcal{H}}{\partial q_i} \dot{q}_i^c + \frac{\partial \mathcal{H}}{\partial p_i} \dot{p}_i^c = -\gamma \sum_i \left(\frac{\partial \mathcal{H}}{\partial p_i}\right)^2. \tag{43}$$

Because the energy along an orbit has to be periodic, the only possibility when $\gamma \neq 0$ is that it is constant and $\frac{\partial \mathcal{H}}{\partial p_i} = 0$. If the Hamiltonian is of the form $\mathcal{H} = \frac{1}{2}\boldsymbol{p}^2 + V(\boldsymbol{q})$, this implies that $p_i^c = 0$ and $q_i^c = \text{constant}$. More generally, this implication has to be verified, but it is true in all but very pathological examples.[7]

For every fixed point x^c, the eigenvalues u_i^c of $U^c(t)$ are

$$u_i^c = e^{-A_i^c t}, \tag{44}$$

where the A_i^c are the (in general complex) eigenvalues of $A_{ij}[x_c]$ (Cf. Eqs. (32) and (36)). The Morse index of such a critical point is the number of eigenvalues such that $|u_i^c| > 1$ or equivalently $\text{Re } A_i^c < 0$. The result of the preceeding section implies on one hand that all the moduli of the eigenvalues of e^{-tH} are to this order in T smaller or equal than one. On the other hand, the number M_k of eigenvalues that are one within the k fermion subspace coincides with the number of critical points of index k.

For large t, we have then:

$$\lim_{t \to \infty} T(\lambda, t) = \lim_{t \to \infty} \sum_k \lambda^k \text{Tr}(e^{-tH})|_{k \text{ ferm.}} = \sum_k \lambda^k M_k, \tag{45}$$

because eigenvalues of e^{-tH} with moduli smaller than one are exponentially suppressed as in ordinary SUSY-QM.

On the other hand,

$$T(\lambda, t) = \sum_{k=0}^{2N} \lambda^k \text{Tr}(e^{-tH})|_{k \text{ ferm.}}$$

$$= \sum_{k=0}^{2N} \lambda^k \text{Tr}(e^{-tH})|_{k \text{ ferm.}}^{\text{unpaired}} + \sum_{k=0}^{2N} \lambda^k \text{Tr}(e^{-tH})|_{k \text{ ferm.}}^{\text{paired}}, \tag{46}$$

where the supraindices denote traces taken over subspaces spanned by "paired" and "unpaired" states, as defined in Section 2.3.2. We now introduce the partial traces:

$$R_k(t) \equiv \text{Tr}(e^{-tH})|_{k \text{ ferm.}}^{\text{paired states anihilated by } \bar{Q}}. \tag{47}$$

---

[7] For instance if the points where $\frac{\partial \mathcal{H}}{\partial p_i} = 0$ are isolated in p_i's direction, then this assertion holds. This is for example the case of $\mathcal{H} = (p - f(q))^2 + V(q)$. In more exotic cases, for instance if the phase space is periodic in p and $\mathcal{H} = f(q)g(p) + h(q)$ with $f(q_0) = f'(q_0) = 0$, the solution corresponding to $q = q_0$ and $p = h'(q_0)t$ is a periodic orbit, which is not localized on a critical points.

Taking into account the pairing of the spectrum (Fig. 1), the fact that the eigenvalues of the unpaired eigenstates are zero and that the dimension of the space they generate gives the Betti numbers (see Section 2.3.2), we get:

$$T(\lambda, t) = \sum_{k=0}^{2N} \lambda^k B_k + \sum_{k=0}^{2N} \lambda^k (R_k(t) + R_{k-1}(t))$$

$$\lim_{t \to \infty} T(\lambda, t) = \sum_{k=0}^{2N} \lambda^k B_k + \sum_{k=0}^{2N} \lambda^k (R_k(\infty) + R_{k-1}(\infty)),$$

(48)

where the $R_k(\infty)$ are integers: the number of paired eigenstates of H annihilated by $\bar{Q}$ having eigenvalue zero to leading order in T. Putting together (45) and (48), we have:

$$M_k = B_k + R_k(\infty) + R_{k-1}(\infty). \tag{49}$$

The positivity of the $R_k(\infty)$ (except for $R_{-1}(\infty) = 0$) constitute the strong Morse inequalities:

$$\forall p \quad \sum_{k=0}^{p} (-1)^k B_{p-k} \le \sum_{k=0}^{p} (-1)^k M_{p-k} \tag{50}$$

It is an easy calculation to show for $\mathcal{H}$ of the form $\frac{1}{2} p^2 + V(q)$ that the index defined here as the number of eigenvalues with negative real parts tends to the usual index defined as the number of negative eigenvalues of the potential V as $\gamma \to 0$.

Before concluding this section, let us remark that all we have done here is valid if γ is kept finite as $T \to 0$. If we wish to consider $\gamma \to 0$ together with $T = 0$, then orbits that are not fixed points contribute. This is most easily seen by considering the action in the path integral of Appendix A, which can be written:

$$S = \frac{1}{2\gamma T} \int dt \left(\dot{p}_i + \gamma \frac{\partial \mathcal{H}}{\partial p_i} - \frac{\partial \mathcal{H}}{\partial q_i} \right)^2 = \frac{1}{2\gamma T} \int dt \left(\dot{p}_i - \frac{\partial \mathcal{H}}{\partial q_i} \right)^2$$

$$+ \frac{\gamma}{2T} \int dt \, \dot{q}_i^2 - \int dt \, \frac{\partial \mathcal{H}}{\partial t}, \tag{51}$$

restricted to periodic trajectories such that $\dot{q}_i = \frac{\partial \mathcal{H}}{\partial p_i}$. If the Hamiltonian is time-independent, the term $\frac{\gamma}{2T} \int dt \, \dot{q}_i^2$ suppresses periodic orbits that are not fixed points. However, if we consider $\gamma \to 0$, $T \to 0$, keeping $\frac{\gamma}{T}$ finite, then non-fixed orbits will contribute, and we may get richer inequalities. We shall not follow this strategy here, although it seems a promising line of research.

5. A WKB APPROACH

In this section we treat a Hamiltonian of the form:

$$\mathcal{H}(\mathbf{q}, \mathbf{p}) = \frac{\mathbf{p}^2}{2} + V(\boldsymbol{q}), \tag{52}$$

with a standard WKB treatment that allows to derive Morse theory with a construction very close to the one in SUSY-QM.

5.1. Conservative Forces

For Langevin processes (without inertia), the Fokker-Plank operator is non-Hermitian but can be brought to a Hermitian form by a symmetric real transformation [7,15], provided the forces are conservative. This is true also for the extension with fermions, and the transformation yields the Hermitian SUSY-QM. In the Kramers case H cannot be brought to a Hermitian form, and part of the difficulty with the proofs comes from there. In this section we shall take a closer look at a case for which the discussion simplifies considerably, that of Hamiltonians of the form (52) for which H reads:

$$H = \sum_{i=1}^{N} \left[-\gamma T \frac{\partial^2}{\partial p_i^2} - \frac{\partial V}{\partial q_i} \frac{\partial}{\partial p_i} - \gamma - \gamma p_i \frac{\partial}{\partial p_i} + \frac{\partial}{\partial q_i} p_i + \gamma b_i^\dagger b_i - a_i^\dagger b_i + \sum_{j=1}^{N} \frac{\partial^2 V}{\partial q_i \partial q_j} b_i^\dagger a_j \right]. \tag{53}$$

One can easily verify that H, Q and $\bar{Q}$ are then related to their adjoint by[8]:

$$H^\dagger = RHR^{-1}, \qquad R\bar{Q}R^{-1} = Q^\dagger, \qquad RQR^{-1} = \bar{Q}^\dagger, \tag{54}$$

where R is a real, Hermitian invertible operator defined as (no summation inside the square brackets):

$$R = R^\dagger = e^{\frac{\mathcal{H}}{T}} P J, \quad \text{where} \quad P|\psi(\mathbf{q}, \mathbf{p})\rangle = |\psi(\mathbf{q}, -\mathbf{p})\rangle,$$
$$J = \prod_i [1 + a_i^\dagger b_i + b_i^\dagger a_i - a_i^\dagger a_i - b_i^\dagger b_i + \gamma a_i^\dagger a_i + (\gamma - 2) a_i^\dagger b_i^\dagger a_i b_i]. \tag{55}$$

Equation (54) implies that

$$\tilde{H} = R^{1/2*} H R^{-1/2*} = (R^{1/2} H R^{-1/2})^\dagger, \tag{56}$$

which means that if $R^{1/2}$ were real, then $\tilde{H}$ would be hermitian. However, this is generically not the case. A weaker result that will allow us to transpose easily most of the structure of the SUSY-QM case will be shown below: R is

---

[8] In fact, this symmetry holds generally for systems with energy symmetric under the reflection of $\mathbf{p}$: $\mathcal{H}(\mathbf{q}, -\mathbf{p}) = \mathcal{H}(\mathbf{q}, \mathbf{p})$ and conservative forces.

positive-definite—and hence $R^{1/2}$ real—*when restricted to the eigenspace of the lowest eigenvectors*.

5.2. Gaussian Development

In the standard SUSY-QM case, it is useful to work in the basis in which H is Hermitian, mainly because in that basis the low-lying eigenvectors peak on saddle-points of the potential. It would seem that the analogous thing to do here is to go to an intermediate basis via $R^{1/2}$. As $R^{1/2}$ is in general non-Hermitian, H is not Hermitian in this basis, only (complex) symmetric ($H^* = H^\dagger$). We shall instead introduce a different basis $|\psi^{hR}\rangle = e^{\frac{\beta \mathcal{H}}{2}} |\psi^R\rangle$ and show that the $|\psi^{hR}\rangle$ whose eigenvalues go to zero with the temperature are finite-variance Gaussians. Let us compute:

$$H' = e^{\frac{\beta\mathcal{H}}{2}} H e^{-\frac{\beta\mathcal{H}}{2}}$$

$$= \sum_{i=1}^{N} \left[-\gamma T \frac{\partial^2}{\partial p_i^2} - \frac{\gamma}{2} + \frac{\gamma}{4T} p_i^2 - \frac{\partial V}{\partial q_i} \frac{\partial}{\partial p_i} + p_i \frac{\partial}{\partial q_i} + \gamma b_i^\dagger b_i - a_i^\dagger b_i \right.$$

$$\left. + \sum_{j=1}^{N} \frac{\partial^2 V}{\partial q_i \partial q_j} b_i^\dagger a_j \right].$$

$$\tag{57}$$

Although H' is not Hermitian, it will be more tractable than the original one. For each saddle point we propose a WKB form for the lowest eigenvectors:

$$|\psi^{hR}\rangle = |\psi_b^{hR}(\boldsymbol{q}, \boldsymbol{p})\rangle \otimes |\psi_f^{hR}\rangle$$

$$= e^{-\frac{1}{2T} [B_{q_i q_j}^c (q_i - q_i^c)(q_j - q_j^c) + B_{p_i q_j}^c p_i (q_j - q_j^c) + B_{p_i p_j}^c p_i p_j]} \otimes |\psi_f^{hR}\rangle.$$

$$\tag{58}$$

In Appendix C we show that the Gaussian so defined has finite variance. This is because the matrix $\boldsymbol{B}$ in (58) is not singular, *as it is for unstable saddle points in the original basis* (reflecting the fact that in this basis the lowest eigenfunctions are *not* concentrated on saddles, see Section 8). We conclude that eigenvectors having eigenvalue zero (to leading order in T) are in this basis, just as in the ordinary SUSY-QM case, Gaussians peaked on saddle points: those with k fermions on saddles of index k. In this case, however, right and left eigenvectors do not coincide.

5.3. Zero-Eigenvalue Subspace

In ordinary SUSY-QM, eigenvectors with exactly zero eigenvalue are annihilated by both Q and $\bar{Q}$. This is evident in the basis in which H is Hermitian and Q the Hermitian conjugate of $\bar{Q}$. In the present case, the proof is slightly more

complicated. We start by writing:

$$RH = Q^\dagger R Q + \bar{Q}^\dagger R \bar{Q}. \tag{59}$$

Clearly, the vectors $|\psi\rangle$ annihilated by H and by RH are the same, and they must satisfy:

$$\langle \psi | RH | \psi \rangle = \langle \psi | Q^\dagger R Q | \psi \rangle + \langle \psi | \bar{Q}^\dagger R \bar{Q} | \psi \rangle = \langle Q\psi | R | Q\psi \rangle + \langle \bar{Q}\psi | R | \bar{Q}\psi \rangle = 0. \tag{60}$$

If R were positive definite, then this would immediately imply that both $Q|\psi\rangle$ and $\bar{Q}|\psi\rangle$ are zero. In fact, as mentioned above, R is *not* positive-definite, but one can show that it is so when restricted to the subspace of eigenvectors whose eigenvalues vanish to leading order in T (a space which obviously contains the eigenstates whose eigenvalues vanish exactly). To show this, we develop $|\psi\rangle$ as in the previous subsection:

$$|\phi\rangle = \sum_c \alpha^c e^{-\frac{\beta\mathcal{H}}{2}} |g^c\rangle \otimes |f^c\rangle, \tag{61}$$

where the sum runs over the critical points 'c' of $V(q)$. $|g^c\rangle$ is the normalized Gaussian centered on the critical point while $|f^c\rangle$ is the corresponding (normalized) fermionic part. Let us compute $\langle \phi | R | \phi \rangle$:

$$\begin{aligned}
\langle \phi | R | \phi \rangle &= \sum_{c,c'} \alpha^c \alpha^{c'*} \langle e^{-\frac{\beta\mathcal{H}}{2}} g^c \otimes f^c | e^{\beta\mathcal{H}} PJ | e^{-\frac{\beta\mathcal{H}}{2}} g^{c'} \otimes f^{c'} \rangle \\
&= \sum_{i,j} \alpha^c \alpha^{c'*} \langle g^c | P | g^{c'} \rangle \langle f^c | J | f^{c'} \rangle.
\end{aligned} \tag{62}$$

Two Gaussians centered on two different critical points do not overlap in the small temperature limit:

$$\langle g^c | P | g^{c'} \rangle = \delta_{c,c'} C^c \quad \text{with} \quad C^c > 0, \tag{63}$$

and the scalar product reduces to:

$$\langle \phi | R | \phi \rangle = \sum_c |\alpha^c|^2 C^c \langle f^c | J | f^c \rangle. \tag{64}$$

It remains to show that the fermion contribution is positive. We can assume that we have diagonalized the matrix of second derivatives of the potential at each saddle point, and for each direction i we have (see Appendix (C)) that either $V_{ii} > 0$, and then

$$\langle f_i^c | J | f_i^c \rangle = 1, \tag{65}$$

or $V_{ii} < 0$ and

$$\langle f_i^c | J | f_i^c \rangle = 2\left[\gamma^2(\gamma + \sqrt{\gamma^2 - 4V_{ii}}) - 2V_{ii}(2\gamma + \sqrt{\gamma^2 - 4V_{ii}}) \right] > 0. \tag{66}$$

We have hence shown that in all cases within this subspace either

$$\langle \phi | R | \phi \rangle > 0 \quad \text{or} \quad | \phi \rangle = 0. \tag{67}$$

which, when applied to (60) implies that eigenvectors with exactly zero eigenvalue are unpaired, just as in SUSY-QM.

Paying the price of a loss of generality, this WKB approach shows in a more intuitive way the organization of the spectrum below the gap. The eigenstates can be seen—in an intermediate basis—as Gaussians centered on critical points. This Gaussian development enables us to show that there is no pairing in the zero eigenvalue eigenspace.

6. TIME DEPENDENT SUSY

In this section we study the Kramers problem with a periodic time-dependent Hamiltonian $\mathcal{H}(\boldsymbol{q}, \boldsymbol{p}, t)$ of period τ. We first introduce the Floquet formalism and extend the supersymmetry of the time-independent case to the time-dependent one. We then briefly show how this formalism allows us to rederive the Lefschetz formula and even prove the strong Morse inequalities when the friction is strong enough to prevent the proliferation of orbits of long periods.

6.1. Generalized Operators

The Fokker-Planck equation associated with the Kramers system can be written:

$$\frac{\partial}{\partial t} | \psi(\boldsymbol{q}, \boldsymbol{p}; t) \rangle = -H_K(\boldsymbol{q}, \boldsymbol{p}; t) | \psi(\boldsymbol{q}, \boldsymbol{p}; t) \rangle. \tag{68}$$

Floquet theory is based on proposing solutions through the ansatz:

$$| \psi(\boldsymbol{q}, \boldsymbol{p}; t) \rangle = | u(\boldsymbol{q}, \boldsymbol{p}; t) \rangle e^{-\lambda t}, \tag{69}$$

where $| u(\boldsymbol{q}, \boldsymbol{p}; t) \rangle$ is periodic of period τ and the imaginary part of λ can be chosen in the first 'Brillouin zone' $[-\frac{\pi}{\tau}, \frac{\pi}{\tau}]$. Equation (68) then becomes:

$$\left(H_K + \frac{\partial}{\partial t} \right) | u(\boldsymbol{q}, \boldsymbol{p}; t) \rangle = \lambda | u(\boldsymbol{q}, \boldsymbol{p}; t) \rangle. \tag{70}$$

An alternative way to introduce the Floquet representation[17] is to start from the stochastic equation. Introducing a variable θ which grows linearly in time, we can write the Langevin Eq. (9) as a system evolving with the

time-independent Hamiltonian $\mathcal{H}(\boldsymbol{q}, \boldsymbol{p}, \theta)$:

$$
\begin{cases}
\dot{q}_i = \dfrac{\partial \mathcal{H}}{\partial p_i} \\[2mm]
\dot{p}_i = -\dfrac{\partial \mathcal{H}}{\partial q_i} - \gamma \dfrac{\partial \mathcal{H}}{\partial p_i} + \sqrt{2\gamma T}\,\eta_i \\[2mm]
\dot{\theta} = 1,
\end{cases}
\tag{71}
$$

with

$$
\theta(0) = 0. \tag{72}
$$

The Eq. (70) leads us to a Kramers operator in the space $(\boldsymbol{q}, \boldsymbol{p}, \theta)$:

$$
\mathbb{H}_K = -\gamma \sum_{i=1}^{N} \frac{\partial}{\partial p_i}\left(T\frac{\partial}{\partial p_i} - \frac{\partial \mathcal{H}}{\partial p_i}\right) + \sum_{i=1}^{N}\left(\frac{\partial \mathcal{H}}{\partial q_i}\frac{\partial}{\partial p_i} - \frac{\partial \mathcal{H}}{\partial p_i}\frac{\partial}{\partial q_i}\right) + \frac{\partial}{\partial \theta}. \tag{73}
$$

To construct the supersymmetry of this operator, we first generalize the operator Q by introducing new fermion operators a_θ and $a_\theta^\dagger$:

$$
\mathbb{Q} \equiv Q - i\,a_\theta \frac{\partial}{\partial \theta} = -i \sum_{i=1}^{N}\left(\frac{\partial}{\partial q_i}a_i + \frac{\partial}{\partial p_i}b_i + \frac{\partial}{\partial \theta}a_\theta\right) - i\frac{\partial}{\partial \theta}a_\theta. \tag{74}
$$

We can then extend $\mathbb{H}_K$ by adding fermion creation and annihilation operators:

$$
\begin{aligned}
\mathbb{H} \equiv \mathbb{H}_K &+ \frac{\partial^2 \mathcal{H}}{\partial q_i \partial q_j}b_i^\dagger a_j + \gamma\frac{\partial^2 \mathcal{H}}{\partial p_i \partial p_j}b_i^\dagger b_j - \frac{\partial^2 \mathcal{H}}{\partial p_i \partial p_j}a_i^\dagger b_j \\[2mm]
&+ \frac{\partial^2 \mathcal{H}}{\partial q_i \partial p_j}(\gamma b_j^\dagger a_i + b_i^\dagger b_j - a_j^\dagger a_i) \\[2mm]
&+ \left(\frac{\partial^2 \mathcal{H}}{\partial q_i \partial \theta} + \gamma\frac{\partial^2 \mathcal{H}}{\partial p_i \partial \theta}\right)b_i^\dagger a_\theta - \frac{\partial^2 \mathcal{H}}{\partial p_i \partial \theta}a_i^\dagger a_\theta.
\end{aligned}
\tag{75}
$$

$\mathbb{H}$ commutes with $\mathbb{Q}$, and we can also construct the other generator of supersymmetry:

$$
\bar{\mathbb{Q}} = -i\left[b_i^\dagger\left(\frac{\partial}{\partial q_i} + \gamma\frac{\partial}{\partial p_i} + \frac{1}{T}\frac{\partial \mathcal{H}}{\partial q_i} + \gamma\frac{1}{T}\frac{\partial \mathcal{H}}{\partial p_i}\right) - a_i^\dagger\left(\frac{\partial}{\partial p_i} + \frac{1}{T}\frac{\partial \mathcal{H}}{\partial p_i}\right) - a_\theta^\dagger\right],
$$

$$
\tag{76}
$$

satisfying:

$$
\bar{\mathbb{Q}}^2 = \mathbb{Q}^2 = 0, \quad T[\mathbb{Q}, \bar{\mathbb{Q}}]_+ = T(\mathbb{Q}+\bar{\mathbb{Q}})^2 = \mathbb{H}. \tag{77}
$$

Let us also note that a_θ is a symmetry:

$$
[\mathbb{H}, a_\theta] = 0, \tag{78}
$$

implying that if $|\psi^R\rangle$ is a right eigenvector of $\mathbb{H}$, then $a_\theta|\psi^R\rangle$ is a degenerate one, or zero. In the following sections, we will use the supersymmetry to study the eigenvectors and use it to derive relations between the number of periodic trajectories.

6.2. Structure of the Spectrum—Quadruplets

We shall prove here that the right eigenvectors are in fact duplicated in the following way: one can build a basis $\{|\psi^0\rangle\} \equiv \{|\phi_i^0\rangle, |\chi_i^0\rangle, |\rho_i^0\rangle\}$ of the space annihilated by a_θ which satisfy (28) and complete it by a degenerate free family $\{|\psi^\theta\rangle\} \equiv \{|\phi_i^\theta\rangle, |\chi_i^\theta\rangle, |\rho_i^\theta\rangle\}$, having non zero component along $a_\theta^\dagger$. This basis
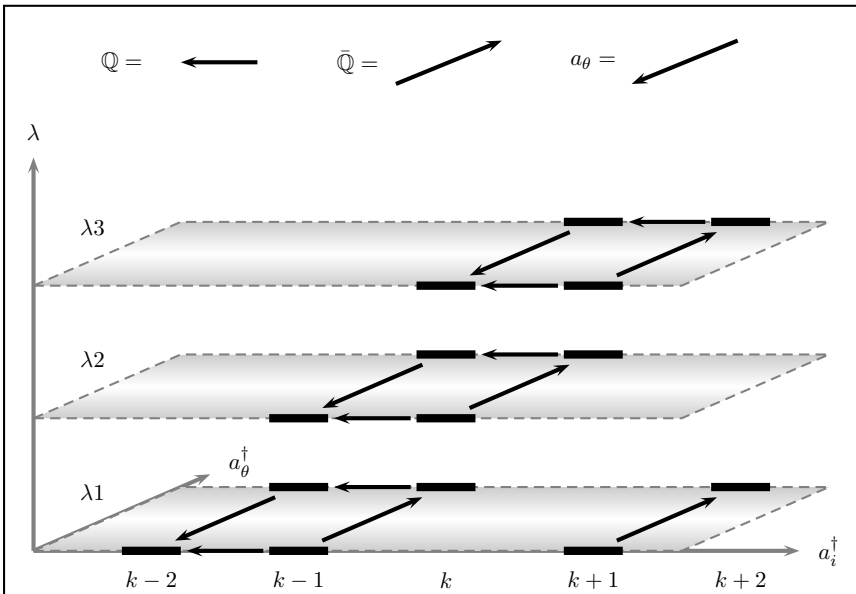

Fig. 3. Structure of the spectrum of $\mathbb{H}$. The vertical axis represents the different complex eigenvalues. The horizontal axes represent the number of fermions of type $a_\theta^\dagger$ and the total number of fermions respectively. One can find a basis of the eigenvectors annihilated by a_θ which is organised as in the time independant case. It can be completed by a degenerate linearly independent family to build a basis of the whole space.

satisfies (see Fig. 3):

$$
\begin{aligned}
&a_\theta |\chi_i^0\rangle = 0 &&a_\theta |\phi_i^0\rangle = 0 &&a_\theta |\rho_i^0\rangle = 0 \\
&a_\theta |\chi_i^\theta\rangle \sim |\chi_i^0\rangle &&a_\theta |\phi_i^\theta\rangle \sim |\phi_i^0\rangle &&a_\theta |\rho_i^\theta\rangle \sim |\rho_i^0\rangle \\
&\mathbb{Q}|\phi_i^0\rangle = |\chi_i^0\rangle &&\mathbb{Q}|\rho_i^0\rangle = 0 &&\forall |\psi\rangle\ Q|\psi\rangle \neq |\rho_i^0\rangle \\
&\bar{\mathbb{Q}}|\phi_i^0\rangle = |\phi_i^\theta\rangle &&\mathbb{Q}|\phi_i^\theta\rangle = |\chi_i^\theta\rangle &&\bar{\mathbb{Q}}|\rho_i^0\rangle = |\rho_i^\theta\rangle
\end{aligned}
\tag{79}
$$

To construct a basis as (79), one first remarks that the procedure followed in Section 2.3.2 is still valid in the subspace annihilated by a_θ. One can thus construct a basis $\{|\rho_i^0\rangle, |\phi_i^0\rangle, |\chi_i^0\rangle\}$ satisfying (28). Next, let us define $\{|\psi^\theta\rangle\}$ as:

$$
\begin{aligned}
|\phi_i^\theta\rangle &\equiv \bar{\mathbb{Q}}|\phi_i^0\rangle = \bar{Q}|\phi_i^0\rangle + \frac{i}{T}a_\theta^\dagger |\phi_i^0\rangle \\[2mm]
|\chi_i^\theta\rangle &\equiv \mathbb{Q}|\phi_i^\theta\rangle = \left(Q\bar{Q} + \frac{1}{T}\frac{\partial}{\partial\theta}\right)|\phi_i^0\rangle - \frac{i}{T}a_\theta^\dagger |\chi_i^0\rangle \\[2mm]
|\rho_i^\theta\rangle &\equiv \bar{\mathbb{Q}}|\rho_i^0\rangle = \bar{Q}|\rho_i^0\rangle + \frac{i}{T}a_\theta^\dagger |\rho_i^0\rangle.
\end{aligned}
\tag{80}
$$

a_θ sends $\{|\psi^\theta\rangle\}$ back to $\{|\psi^0\rangle\}$ (up to constant factors), which proves that $\{|\psi^\theta\rangle\}$ is an independent family. The whole family is obviously also independent, it can generate any vector annihilated by a_θ, thanks to the family $\{|\psi^0\rangle\}$, in particular it can generate the family $\{|\psi^0\rangle, |a^\dagger\psi^0\rangle\}$ which is a basis of the whole space.

Let us look at the $\{|\rho_i^0\rangle\}$. They are annihilated by Q but not the image by Q of any other eigenvector. The dimension of the space generated by such eigenvectors in the k fermion sector is the kth Betti number B_k of the phase space $\{p, q\}$ (see Section 2.3.2). The dimension of the space generated by $\{|\rho_i^0\rangle\}$ in the k fermion sector is then equal to B_{k-1} (see Fig. 3).

In the following, we will call "paired" states and "unpaired" states, the eigenvectors generated by $\{|\chi_i^0\rangle, |\phi_i^0\rangle, |\chi_i^\theta\rangle, |\phi_i^\theta\rangle\}$ and $\{|\rho_i^0\rangle, |\rho_i^\theta\rangle\}$, respectively.

As in any Floquet problem, the spectrum is organized in Brillouin zones. This can be seen directly as follows. Consider the family of periodic operators $O_m = e^{2\pi i m\theta/\tau}$ with m integer. Clearly, $[\mathbb{H}, O_m] = 2\pi i m\, O_m$, which implies that if $|\psi^R\rangle$ is an eigenvector with eigenvalue λ then $O_m|\psi^R\rangle$ is an eigenvector with eigenvalue $\lambda + 2\pi i m$. This redundancy is eliminated if we consider the operator $e^{-n\tau\mathbb{H}}$ restricted to a particular starting point for θ:

$$
\mathrm{Tr}\left(\langle\theta = n\tau \left| e^{-n\tau\mathbb{H}}\right| \theta = 0\rangle\right)\Big|^{\text{other}} = \mathrm{Tr}\left[\mathcal{T}e^{\int_0^{n\tau} H(t)dt}\right].
\tag{81}
$$

where 'other' means that the trace is taken over all variables (including fermions) except θ, and $H(t)$ is:

$$H(t) \equiv -\frac{\partial}{\partial p_i}\left(\gamma T \frac{\partial}{\partial p_i} + \frac{\partial \mathcal{H}}{\partial q_i} + \gamma \frac{\partial \mathcal{H}}{\partial p_i}\right) + \frac{\partial}{\partial q_i}\frac{\partial \mathcal{H}}{\partial p_i} + \frac{\partial^2 \mathcal{H}}{\partial q_i \partial q_j} b_i^\dagger a_j$$

$$+ \gamma \frac{\partial^2 \mathcal{H}}{\partial p_i \partial p_j} b_i^\dagger b_j - \frac{\partial^2 \mathcal{H}}{\partial p_i \partial p_j} a_i^\dagger b_j + \frac{\partial^2 \mathcal{H}}{\partial q_i \partial p_j}(\gamma b_j^\dagger a_i + b_i^\dagger b_j - a_j^\dagger a_i) \quad (82)$$

$$+ \left(\frac{\partial^2 \mathcal{H}}{\partial q_i \partial t} + \gamma \frac{\partial^2 \mathcal{H}}{\partial p_i \partial t}\right) b_i^\dagger a_\theta - \frac{\partial^2 \mathcal{H}}{\partial p_i \partial t} a_i^\dagger a_\theta.$$

6.3. Trace of the Evolution Operator

Let us start by building a generating function just as in the previous section. We fix the starting point at $\theta = 0$ and compute the trace:

$$T(\lambda, n\tau) \equiv \sum_k \lambda^k \text{Tr}\left(\langle\theta = n\tau \left| e^{-n\tau\mathbb{H}} \right| \theta = 0\rangle\right)\Big|_{k \text{ ferm}}^{\text{other}}$$

$$= \sum_k \lambda^k \text{Tr}\left(\mathcal{T} e^{\int_0^{n\tau} H(t)dt}\right)|_{k \text{ ferm}}, \quad (83)$$

where 'other' again means that the trace is over all the variables except θ. In the k fermion sector, it is divided in two parts:

$$T_k = \text{Tr}\left(\mathcal{T} e^{-\int_0^{n\tau} H(t)\,dt}\right)\Big|_{k \text{ ferm.}} = \text{Tr}\left(\mathcal{T} e^{-\int_0^{n\tau} H(t)\,dt}\right)\Big|_{k \text{ ferm.}}^{\text{unpaired}}$$

$$+ \text{Tr}\left(\mathcal{T} e^{-\int_0^{n\tau} H(t)\,dt}\right)\Big|_{k \text{ ferm.}}^{\text{paired}}. \quad (84)$$

Let us show that unpaired eigenvectors have eigenvalue 0. Suppose that $H|\rho_i^0\rangle = \lambda|\rho_i^0\rangle$ with λ not an integer multiple of $i\frac{2\pi}{\tau}$, that is, $\lambda \neq 0$ inside the first Brillouin zone. As Q and a_θ annihilate $|\rho_i^0\rangle$:

$$\frac{1}{T}H|\rho_i^0\rangle = \mathbb{Q}\bar{\mathbb{Q}}|\rho_i^0\rangle = \frac{\lambda}{T}|\rho_i^0\rangle. \quad (85)$$

Since $\mathbb{Q} = Q - i a_\theta \frac{\partial}{\partial\theta}$, (85) can be written

$$Q\bar{\mathbb{Q}}|\rho_i^0\rangle = \left(\lambda - \frac{\partial}{\partial\theta}\right)|\rho_i^0\rangle. \quad (86)$$

Because λ is not zero inside the first Brillouin zone, $\mathcal{O} \equiv \lambda - \frac{\partial}{\partial\theta}$ acting on periodic functions of θ is invertible. As $[Q, \mathcal{O}] = 0$, one also has $[Q, \mathcal{O}^{-1}] = 0$. (86) then

reads

$$Q\left(\frac{T}{\lambda}\mathcal{O}^{-1}\bar{\mathbb{Q}}|\rho_i^0\rangle\right) = |\rho_i^0\rangle, \tag{87}$$

which contradicts the fact that $|\rho_i^0\rangle$ is unpaired by Q. This shows that the unpaired eigenstates have eigenvalues zero, and the trace over them simply gives their number:

$$\text{Tr}\left(\mathcal{T}\,e^{-\int_0^{n\tau} H(t)\,dt}\right)\Big|_{k\text{ ferm.}}^{\text{unpaired}} = B_k + B_{k-1} \tag{88}$$

so that:

$$T(\lambda, n\tau) = (1+\lambda)\sum_{k=0}^{2N}\lambda^k B_k + \sum_k \lambda^k \text{Tr}\left(\mathcal{T}\,e^{-\int_0^{n\tau} H(t)\,dt}\right)\Big|_{k\text{ ferm.}}^{\text{paired}}. \tag{89}$$

On the other hand, because of the quartet structure,

$$\text{Tr}\left(\mathcal{T}\,e^{-\int_0^{n\tau} H(t)\,dt}\right)\Big|_{k\text{ ferm.}}^{\text{paired}} = \text{Tr}\left(\mathcal{T}\,e^{-\int_0^{n\tau} H(t)\,dt}\right)\Big|_{k\text{ ferm.}}^{\text{paired without }a_\theta^\dagger}$$
$$+ \text{Tr}\left(\mathcal{T}\,e^{-\int_0^{n\tau} H(t)\,dt}\right)\Big|_{k\text{ ferm.}}^{\text{paired with }a_\theta^\dagger}, \tag{90}$$

leading to (see Fig. 3):

$$T(\lambda, n\tau) = (1+\lambda)\sum_{k=0}^{2N}\lambda^k B_k + (1+\lambda)\sum_k \lambda^k \text{Tr}\left(\mathcal{T}\,e^{-\int_0^{n\tau} H(t)\,dt}\right)\Big|_{k\text{ ferm.}}^{\text{without }a_\theta}$$

$$T(\lambda, n\tau) = (1+\lambda)\sum_{k=0}^{2N}\lambda^k B_k + (1+\lambda)\sum_{k=0}^{2N}\lambda^k (R_k(n\tau) + R_{k+1}(n\tau)). \tag{91}$$

where again we have denoted $R_k(n\tau)$ the partial trace of $e^{-n\tau\mathbb{H}}$ over k-fermion states annihilated by a_θ and not by $\mathbb{Q}$.

We now perform the low temperature 'semi-classical' evaluation of the trace. Because we only need the trace restricted to states without a_θ, all the calculation in Section 3 carries through without modifications, since the last two terms in (82) that are absent in (12) vanish in this subspace. We have then:

$$T(\lambda, n\tau) = \sum_k \lambda^k \text{Tr}\left(\mathcal{T}e^{\int_0^{n\tau} H(t)dt}\right)\Big|_{k\text{ ferm}}$$

$$= (1+\lambda)\sum_k \lambda^k \text{Tr}\left(\mathcal{T}e^{\int_0^{n\tau} H(t)dt}\right)\Big|_{k\text{ ferm}}^{\text{without}\theta} \tag{92}$$

$$\xrightarrow[T\to 0]{} (1+\lambda)\sum_{\substack{\text{noiseless}\\\text{orbits c}}} \frac{\det(1+\lambda U^c(n\tau))}{|\det(1-U^c(n\tau))|}.$$

so that, finally:

$$\sum_{\substack{\text{noiseless} \\ \text{orbits c}}} \frac{\det(1 + \lambda U^c(n\tau))}{|\det(1 - U^c(n\tau))|} = \sum_{k=0}^{2N} \lambda^k B_k + \sum_{k=0}^{2N} \lambda^k (R_k(n\tau) + R_{k+1}(n\tau)). \quad (93)$$

For $\lambda = -1$, this gives the Lefschetz formula. For any n:

$$\sum_{\substack{\text{noiseless} \\ \text{orbits } c}} \text{sign}(\det(1 - U^c(n\tau))) = \sum_{k=0}^{2N} (-1)^k B_k. \quad (94)$$

We can also obtain strong Morse inequalities for the case in which the total number of orbits is finite. This will happen if the friction is sufficiently strong and the time dependent forces are sufficiently weak.

Consider first the case in which there are only orbits of period τ (e.g. the case of a dissipative, adiabatic evolution). We concentrate on an orbit and its corresponding $U^c(\tau)$ with eigenvalues $u_{i_1}, \ldots, u_{i_{2N}}$. We order them so that $u_{i_1} \ldots u_{i_r}$ verify $|u_{i_j}| > 1$ and $u_{i_{r+1}}, \ldots, u_{i_{2N}}$ verify $|u_{i_j}| < 1$, by definition the Morse index of the trajectory is then equal to r. We compute for large n the l.h.s. of (93):

$$\frac{\det(1 + \lambda U^c(n\tau))}{|\det(1 - U^c(n\tau))|} = \sum_k \lambda^k \sum_{j_1, \ldots, j_k} \frac{u_{j_1}^n \ldots u_{j_k}^n}{\prod_{i=1}^{2N} |1 - u_i^n|} \underset{n \to \infty}{\sim} \sum_k \lambda^k \sum_{j_1, \ldots, j_k} \frac{u_{j_1}^n \ldots u_{j_k}^n}{|u_{i_1}^n \ldots u_{i_r}^n|} = \lambda^r. \quad (95)$$

since the only contribution which survives corresponds to $\{j_1, \ldots, j_k\} = \{i_1, \ldots, i_r\}$.[9]

In the limit $n \to \infty$, (93) then becomes:

$$\sum_{k=0}^{2N} \lambda^k B_k + \sum_k \lambda^k (R_{k+1}(\infty) + R_k(\infty)) = \sum_k \lambda^k M_k, \quad (96)$$

where M_k is the number of orbits with Morse index k, and $R_k(\infty)$ the number of eigenstates of $\mathbb{H}$ having zero eigenvalue (to this order in T) annihilated by a_θ and not by $\mathbb{Q}$.

Although we know of no concrete example, let us now outline how equation (96) would be derived for a system with a *finite* number of periodic orbits of several different periods. Consider again the limit of large n, but taken for n prime. The path-integral evaluation of the trace tells us that we have to sum the contributions of all orbits of period $n\tau$, that is, the repetitions of n times the orbit of period τ. On the other hand, as we have seen above, the spectrum of $\mathcal{T} e^{-\int_0^\tau H(t)dt}$ contains, in the presence of orbits of prime period $= p\tau$, multiplets proportional (to this order)

---

[9] We are assuming again that the number of real eigenvalues $u_i < -1$ is even, otherwise the contribution is $-\lambda^r$.

to a number times the p different roots of unity, and their contribution disappears from the trace over n cycles, since n is not a multiple of p. Hence, formula (96) is still valid, but now the $R_k(\infty)$ counts only the eigenstates of $\mathbb{H}$ having zero eigenvalue (to this order in T) annihilated by a_θ and not by $\mathbb{Q}$ that are not part of a multiplet.

The fact that the $R_k(\infty)$ are positive integers in equation (96) constitute the strong Morse inequalities, valid for relatively large γ and/or small intensity of the time-dependent potential so that there is a finite total number of periodic orbits.

7. STOCHASTIC DYNAMICS IN THE K-FERMION SECTOR

In this section we describe a stochastic dynamics that corresponds to the extension of the Kramers equation to evolution of vectors with k fermions. We restrict ourselves to the case in which $\mathcal{H}$ is time-independent, although the generalization is straightforward. The purpose of this exercise is twofold: first, as we shall discuss below, we intend to use this dynamics as a practical method to find reaction paths and other structures in phase-space, and second, we shall use the equations obtained to construct explicitly the low-temperature eigenvectors in the k-fermion subspace, thus completing Morse Theory. In fact, the derivation is practically identical to the one for SUSY-QM in.[7]

We wish to find a stochastic process such that it somehow represents

$$\frac{\partial}{\partial t}|\psi_k(\boldsymbol{x}, t)\rangle = -H|\psi_k(\boldsymbol{x}, t)\rangle, \tag{97}$$

where $|\psi_k(\boldsymbol{x}, t)\rangle$ has k fermions. For large times, the $|\psi_k(\boldsymbol{x}, t)\rangle$ will be a combination of states whose eigenvalues have small real parts.

For zero fermions the dynamics associated with (97) is clearly Hamiltonian + noise + friction. Let us discuss the one-fermion sector in some detail. A one-fermion wavefunction has the form $\psi_i(\boldsymbol{x})c_i^\dagger|-\rangle$, in phase-space variables. Equation (97) reads, for the components $\psi_i(\boldsymbol{x})$:

$$\frac{\partial}{\partial t}\psi_i(\boldsymbol{x}, t) = -H_K\psi_i(\boldsymbol{x}, t) - A_{ij}\psi_j(\boldsymbol{x}, t). \tag{98}$$

Consider first one particle with a $2N$-component normalized vector $\boldsymbol{u}$ attached to it. The position of the particle evolves as a Langevin process (9), and the vector $\boldsymbol{u}$ as:

$$\dot{u}_i = -A_{ij}u_j + N(\boldsymbol{u})u_i, \tag{99}$$

where $N(\boldsymbol{u}) = \sum_{kl} u_k A_{kl}u_l$ enforces the constancy of the norm $\sum_i u_i^2 = 1$. The only effect of the vector $\boldsymbol{u}$ on the dynamics is that we further impose that each particle has a creation-annihilation average rate $= N(\boldsymbol{u})$. From (9) and (99), we

have that the joint distribution function $\mathcal{F}(\boldsymbol{x}, \boldsymbol{u}, t)$ evolves then as:

$$\frac{\partial \mathcal{F}}{\partial t} = \left[-H_K - N(\boldsymbol{u}) + \sum_i \frac{\partial}{\partial u_i} \left(\sum_j A_{ij} u_j - N(\boldsymbol{u}) u_i \right) \right] \mathcal{F}. \tag{100}$$

One can check, using integration by parts, that

$$\psi_i(\boldsymbol{q}, t) = \int d^N \boldsymbol{u} \; u_i \; \mathcal{F}(\boldsymbol{q}, \boldsymbol{u}, t) \tag{101}$$

will evolve according to (98).

The k-fermion generalization is straightforward. The dynamics (97) for a vector

$$\boldsymbol{\psi} = \sum_{i_1,\dots,i_k} \psi_{i_1,\dots,i_k}(\boldsymbol{x}) c_{i_1}^\dagger \dots c_{i_k}^\dagger |-\rangle, \tag{102}$$

where the $\psi_{i_1,\dots,i_k}(\boldsymbol{x})$ are totally antisymmetric, reads, in components:

$$\dot{\psi}_{i_1,\dots,i_k} = -H_K \psi_{i_1,\dots,i_k} - \sum_\sigma \sum_\alpha (-1)^{n(\sigma,\alpha)} A_{\sigma(i_1),\alpha} \; \psi_{\sigma(i_2),\dots,\alpha,\dots,\sigma(i_k)}, \tag{103}$$

where σ denotes all permutations of k indices, and $n(\sigma, \alpha)$ is the sign of the permutation $(i_1, i_2, \dots, \alpha, \dots, i_k) \to (\alpha, \sigma(i_1), \sigma(i_2), \dots, \sigma(i_k))$. Again, the particles follow equation (9), while the equations of motion for the $\boldsymbol{v}$ read:

$$\dot{v}_{i_1,\dots,i_k} = -\sum_\sigma \sum_\alpha (-1)^{n(\sigma,\alpha)} A_{\sigma(i_1),\alpha} \; v_{\sigma(i_2),\dots,\alpha,\dots,\sigma(i_k)} + v_{i_1,\dots,i_k} \; \mathcal{N}(\boldsymbol{v}), \tag{104}$$

with

$$\mathcal{N}(\boldsymbol{v}) = \sum_{i_1,\dots,i_k} v_{i_1,\dots,i_k} \sum_\sigma \sum_\alpha (-1)^{n(\sigma,\alpha)} A_{\sigma(i_1),\alpha} \; v_{\sigma(i_2),\dots,\alpha,\dots,\sigma(i_k)}, \tag{105}$$

thus preserving the normalization $\sum_{i_1,\dots,i_k} v_{i_1,\dots,i_k}^2$. As before, there is cloning with rate $\mathcal{N}(\boldsymbol{v})$. It is easy to see that average of $v_{i_1,\dots,i_k}$ indeed evolves as the $\psi_{i_1,\dots,i_k}(\boldsymbol{x})$.

The equations of motion for $(\boldsymbol{v}, \mathcal{N}(\boldsymbol{v}))$ give the expansion rate of a volume element driven by the dynamics. Given a point $\boldsymbol{x}$, we can write a volume element around it as:

$$V^k = \delta \boldsymbol{x_1} \wedge \delta \boldsymbol{x_2} \wedge \dots \wedge \delta \boldsymbol{x_k} \equiv \mathcal{M} \sum_{v_{i_1,\dots,i_k}} v_{i_1,\dots,i_k} \hat{e}_{i_1} \wedge \dots \wedge \hat{e}_{i_k}, \tag{106}$$

where $\wedge$ is the external (wedge) product, $\hat{e}_i$ are the basis vectors and the form $v_{i_1,\dots,i_k}$ is normalized. The orientation and norm of the volume element evolve along a trajectory of the particle. Equation (104) gives the evolution of the orientation $\boldsymbol{v}$, and $\mathcal{N} = \dot{\mathcal{M}}$ gives the expansion rate.

Low-lying eigenstates of H and geometric structures. The right eigenvectors $\langle x|\psi_a^R\rangle$ with 'low' eigenvalues—with real part going to zero in the limit $T \to 0$—are concentrated on the following structures:

- For $k = 0$: local minima.
- For $k = 1$: paths originating in saddles of index one, spiralling down (thanks to friction) to local minima.
- For any k: the k-dimensional surface generated by all paths decreasing in energy emanating from a saddle of index k.

The argument is the same as in the purely dissipative SUSY-QM case[7]: we consider that the surface descending from the saddle of index k is uniformly covered with particles with their k-form v at each point tangential to such a surface. Both features are preserved by the evolution, as seen in the previous subsection. First, as the particles go downhill, the v attached to them change so as to remain tangential: this is because their evolution are precisely based on the linearized evolution on the tangent space. Secondly, the cloning rate matches exactly the expansion rate of a small volume advected downhill. Hence, the distribution of particles descending, and the average value of the forms $v_{i_1,\ldots,i_k}$ attached to them is left invariant by the $T = 0$ dynamics.

8. TRANSITION PATHS. 'REDUCED CURRENT'

Part of the motivation for this work has been to use the higher fermion subspaces to find useful information on phase-space. In particular, in the Fokker-Planck SUSY-QM case, the low-lying eigenvectors of the one fermion subspace yield the transition currents between states. Here, as we shall see, the formalism itself tells us that, in order to compute the transition path, the relevant quantity is a 'reduced current', rather than the usual one. Consider first the Kramers equation (10):

$$\frac{\partial P(\mathbf{q}, \mathbf{p}, t)}{\partial t} = -H_K P(\mathbf{q}, \mathbf{p}, t) = -\mathrm{div}\, \boldsymbol{J} = -\left(\frac{\partial J_{q_i}}{\partial q_i} + \frac{\partial J_{p_i}}{\partial p_i}\right), \qquad (107)$$

which defines the current:

$$J_{q_i} = \frac{\partial \mathcal{H}}{\partial p_i} P(\mathbf{q}, \mathbf{p}, t) \quad J_{p_i} = -\left(\gamma T \frac{\partial}{\partial p_i} + \gamma \frac{\partial \mathcal{H}}{\partial p_i} + \frac{\partial \mathcal{H}}{\partial q_i}\right) P(\mathbf{q}, \mathbf{p}, t). \quad (108)$$

Inspired by the Langevin/Fokker-Planck case, we apply the operator $\bar{Q}$ to a distribution to obtain a current. We get:

$$(-i)T\ \bar{Q} P(\mathbf{q}, \mathbf{p}, t) = |\psi^R\rangle \equiv J_{q_i}^{\mathrm{red}} a_i^\dagger |-\rangle + J_{p_i}^{\mathrm{red}} b_i^\dagger |-\rangle, \qquad (109)$$
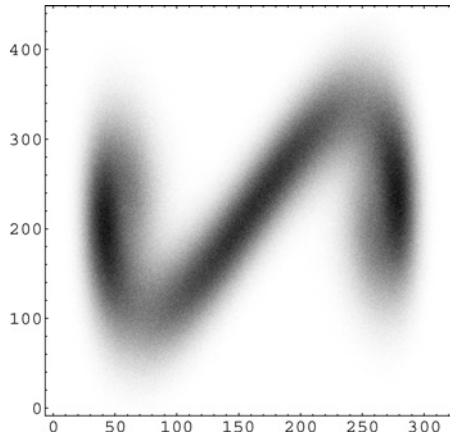
Fig. 4. Reduced current for the double-well potential of Section 8. One can see that the structure is concentrated on two damped paths, starting in the saddle point, and spiralling down to the two minima, respectively. The width of the structure is $\sim \sqrt{\gamma T}$.

where we have defined the *reduced current* as:

$$J_{q_i}^{\mathrm{red}} \equiv J_{q_i} + T \frac{\partial P(\mathbf{q}, \mathbf{p})}{\partial p_i} \quad J_{p_i}^{\mathrm{red}} = J_{p_i} - T \frac{\partial P(\mathbf{q}, \mathbf{p})}{\partial q_i}. \tag{110}$$

The reduced current has the following good properties:

- It differs from the current in a term without divergence, hence the fluxes over closed surfaces coincide.
- It is zero in equilibrium. In a case with metastable states, it is small everywhere, while the true current is large within the states.

It is easy to prove that $\bar{Q}$ is the only first-order differential operator that gives a 'current' field with the same fluxes as the standard current while being zero when applied to the equilibrium Gibbs state.

In the Fokker-Planck SUSY-QM case, the supersymmetry allows us to obtain the usual transition current on the basis of 1-fermion low lying states. Here, the supersymmetric formalism itself has suggested a new definition for the current, and a practical way to determine it (on the basis of simulating equation (98)). The reduced current is more relevant than the total one as it is directly related to passages rather than to phase space orbits within a state.

An example. The example which we have studied is that of one particle evolving in the one-dimensional double-well potential $V(q) = (q^2 - 1)^2$. We have
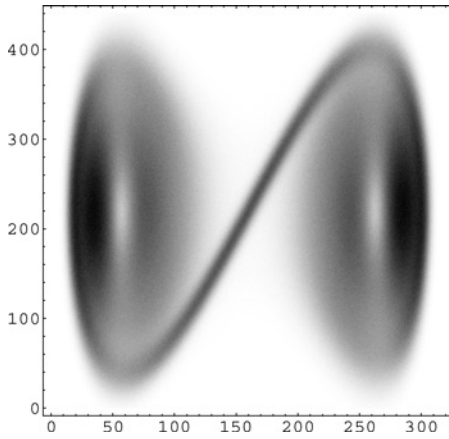
Fig. 5. Same as Fig. 4, with smaller damping.

carried out simulations using the algorithm presented in the Section 7 and compared it with a determination of the current by direct simulation, see Figs. 4 and 5.[10]

9. CONCLUSION AND PERSPECTIVES

We have shown how the supersymmetry associated with the Kramers equation can be used to extract results of Morse theory in an elementary way. The strategy is very close to the one followed for the SUSY-quantum mechanics case, although somewhat complicated by the fact that the operators are non-Hermitian. Compared to the case of pure Hamiltonian dynamics, we have here a term of friction $\propto \gamma$, and a term of noise $\propto \sqrt{\gamma T}$ which we can take to zero in several ways. Thanks to them, the Hilbert space on which the evolution operator acts is well defined, and the spectra of the operators are discrete. The wavefunctions associated with the eigenvalues with real part close to zero are concentrated on the structures associated with Morse Theory.

The same methods can be used for a periodically time-dependent system, using a supersymmetric structure acting in the Floquet representation of the problem. The program for this case is however far from complete, below we mention some possible continuations.

---

[10] The numerical simulation of the Eq. (1), especially in the low friction limit, should be implemented carefully, as a finite integration step will produce large errors. We have used quasi simplectic integrators (see[22] and references therein) which provide reliable results in the whole range of friction we studied.

The advantage of this formulation is not only that it is entirely contained in (physics) undergraduate level, but that it makes a connection with situations of interest in physics and physical chemistry. Although we have used the low-temperature limit as a way to make the wavefunctions peak on saddles and other structures, other limiting situations yielding time scale-separation could have been invoked. For example, in many macroscopic systems, the thermodynamic states become mutually inaccessible (or almost), and thus play the same role as minima in the low-temperature case. The formalism applied here can then be used to build a Morse Theory for states, their transition currents, and higher objects. The practical determination of metastable states and transition paths in this wider context is an active field of research, especially in complex energy landscapes relevant for chemical reactions.

We have not dealt here with two elements that are needed in order to go beyond:

- Degenerate Morse Theory, non-isolated orbits.
- Proliferating orbits

Degenerate solutions appear in a time-independent system as soon as we have to consider orbits rather than fixed points, corresponding to the freedom of choosing the starting point of the orbit. This degeneracy has already been discussed in the case of SUSY-QM,[2] and although it makes the treatment more cumbersome, it is a rather standard exercise in collective coordinates. Two cases when orbits arise naturally in a time-independent system are when forces do not derive from a global potential (like a magnetic monopole subjected to a magnetic field), or when the friction is scaled to zero with the temperature (e.g. γ/T finite).

In systems for which the number of orbits grows exponentially with the period, a finer method of classifying orbits than the one used in this paper has to be put in place. This is the subject of Floer Theory, which we have only marginally touched.

One last development that has been left out here is the case of Hamiltonian systems with no friction but with thermal noise (for such an infinite temperature situation, the phase-space has to be finite). Let us just remark here that in the corresponding low-noise limit, the supersymmetric formalism provides a method to study the separatrices and homoclinic orbits.

APPENDIX A

The generating function of the evolution operator can be written in path integral formalism as[18]:

$$
T(\lambda, t) \equiv \mathrm{Tr}\big(\lambda^F \mathcal{T} e^{-\int H(t')dt'}\big) = \int_{q_0}^{q_0} \mathcal{D}[\boldsymbol{q}, \boldsymbol{p}, \boldsymbol{\eta}]\, \delta\left(\dot{p}_i + \gamma\, \frac{\partial \mathcal{H}}{\partial p_i} + \frac{\partial \mathcal{H}}{\partial q_i} - \eta_i(t)\right)
$$

$$
\delta\left(\dot{q}_i - \frac{\partial \mathcal{H}}{\partial p_i}\right)\, \exp\left(-\frac{1}{4\,\gamma\,T}\int \sum_i \eta_i^2(t')dt'\right) W[q_j, p_j; t'],
$$

(A1)

where W is defined by:

$$
W[\boldsymbol{q}(t), \boldsymbol{p}(t); t'] = \int \mathcal{D}[\boldsymbol{c}, \bar{\boldsymbol{c}}] e^{-\int dt\, \bar{c}_i\left(\delta_{ij}(\frac{d}{dt} - \ln\lambda) + A_{ij}[\boldsymbol{p}, \boldsymbol{q}]\right)c_i},
$$

(A2)

and $(\bar{c}_j, c_j)$ are Grassmann variables. Using the Fourier representation of the δ function [18], one gets:

$$
T(\lambda, t) = \int_{q_0}^{q_0} \mathcal{D}[\boldsymbol{q}, \hat{\boldsymbol{q}}, \boldsymbol{p}, \hat{\boldsymbol{p}}, \boldsymbol{\eta}] e^{\int_0^t dt'[\hat{p}_i(\dot{p}_i + \gamma \frac{\partial \mathcal{H}}{\partial p_i} + \frac{\partial \mathcal{H}}{\partial q_i} - \eta_i(t)) - \frac{1}{4\gamma T}\sum_i \eta_i^2(t') + \hat{q}_i(\dot{q}_i - \frac{\partial \mathcal{H}}{\partial p_i})]}
$$

$$
\times\; W(\boldsymbol{q}, \boldsymbol{p}; t).
$$

(A3)

The question of factor ordering can be dealt with by choosing a convention in which the integral above represents the Kramers dynamics. In our case we need not worry about this, as we will only use the path integral as a bookkeeping device. The integration over the noise results in:

$$
T(\lambda, t) = \int_{q_0}^{q_0} \mathcal{D}[\boldsymbol{q}, \hat{\boldsymbol{q}}, \boldsymbol{p}, \hat{\boldsymbol{p}}]\, e^{\int dt'[\hat{p}_i(\dot{p}_i + \gamma \frac{\partial \mathcal{H}}{\partial p_i} + \frac{\partial \mathcal{H}}{\partial q_i}) + \hat{p}_i^2 \gamma\, T + \hat{q}_i(\dot{q}_i - \frac{\partial \mathcal{H}}{\partial p_i})]} W(\boldsymbol{q}, \boldsymbol{p}; t).
$$

(A4)

Integration over $\hat{\boldsymbol{p}}$ and $\hat{\boldsymbol{q}}$ gives a 'Lagrangian' version of the path-integral:

$$
T(\lambda, t) = \int_{q_0}^{q_0} \mathcal{D}[\boldsymbol{q}, \boldsymbol{p}] e^{-\frac{1}{4\gamma T}\int dt'(\dot{p}_i + \gamma \frac{\partial \mathcal{H}}{\partial p_i} + \frac{\partial \mathcal{H}}{\partial q_i})^2}\, \delta\left(\dot{q}_i - \frac{\partial \mathcal{H}}{\partial p_i}\right) W(\boldsymbol{q}, \boldsymbol{p}; t). \quad \text{(A5)}
$$

The factor $1/\gamma T$ multiplying the action becomes large when the temperature goes to zero, and the path integral is then dominated by periodic orbits satisfying:

$$
\begin{cases}
\dot{p}_i^c = -\dfrac{\partial \mathcal{H}}{\partial q_i} - \gamma\, \dfrac{\partial \mathcal{H}}{\partial p_i} \\[2mm]
\dot{q}_i^c = \dfrac{\partial \mathcal{H}}{\partial p_i}.
\end{cases}
\qquad \text{(A6)}
$$

One can linearize Eq. (A4) around such an orbit by putting $x_i = x_i^c + \sqrt{T} x_i'$, $\hat{x}_i = \frac{1}{\sqrt{T}} \hat{x}_i'$ and consequently:

$$\frac{\partial \mathcal{H}}{\partial x_i} = \frac{\partial \mathcal{H}}{\partial x_i}\bigg|_{q^c, p^c} + \sqrt{T}\, x_j' \, \frac{\partial^2 \mathcal{H}}{\partial x_i \partial x_j}\bigg|_{q^c, p^c}. \tag{A7}$$

One then gets for the contribution of the orbit to this order:

$$T^c(\lambda, t) =$$

$$\times \int \mathcal{D}[q', \hat{q}, p', \hat{p}]\, e^{-\int dt\, \hat{p}_i (\dot{p}_i' + \gamma\, p_j' \frac{\partial^2 \mathcal{H}}{\partial p_i \partial p_j}|_{q^c, p^c} + \gamma\, q_j' \frac{\partial^2 \mathcal{H}}{\partial p_i \partial q_j}|_{q^c, p^c} + p_j' \frac{\partial^2 \mathcal{H}}{\partial q_i \partial p_j}|_{q^c, p^c} + q_j' \frac{\partial^2 \mathcal{H}}{\partial q_i \partial q_j}|_{q^c, p^c} + \gamma\, \hat{p}_i)},$$

$$e^{-\int dt\, \hat{q}_i (\dot{q}_i' - p_j' \frac{\partial^2 \mathcal{H}}{\partial p_i \partial p_j}|_{q^c, p^c} - q_j' \frac{\partial^2 \mathcal{H}}{\partial p_i \partial q_j}|_{q^c, p^c})}\, W(q^c, p^c; t) \tag{A8}$$

(the leading contribution to the action vanishes). Following our conventions for factor ordering, one recognizes the path integral representation of the trace of the evolution operator associated with the time-dependent harmonic Hamiltonian (31).

APPENDIX B

We now compute the trace corresponding to the bosonic degrees of freedom. Let us assume that the probability distribution is Gaussian:

$$P(\boldsymbol{X}, t) = \exp\left(-\frac{1}{2}\, B_{ij}(t)\big(X_i - X_i^0(t)\big)\big(X_j - X_j^0(t)\big) + C(t)\right), \tag{B1}$$

where $X_i^0(t)$ has to be determined and $C(t)$ is just a normalization factor. $P(\boldsymbol{X}, t)$ evolves with (31):

$$\frac{\partial P}{\partial t} = \frac{\partial}{\partial x_k}\left(D_{kj}\frac{\partial}{\partial x_j} + A_{kj}^c x_j\right) P, \tag{B2}$$

which gives:

$$\frac{\partial P}{\partial t} = \Big[(X_i - X_i^0)(X_j - X_j^0)(BDB - BA^c)_{ij} - (X_i - X_i^0)X_j^0 B A_{ij}^c - D B_{kk} + A_{kk}^c\Big]P. \tag{B3}$$

On the other hand, differentiating directly (B1), we get:

$$\frac{\partial P}{\partial t} = P\left[-\frac{\dot{B}_{ij}}{2}(X_i - X_i^0)(X_j - X_j^0) + B_{ij}\dot{X}_i^0(X_j - X_j^0) + \dot{C}(t)\right]. \tag{B4}$$

Equating (B3) and (B4):

$$\begin{cases} -\dot{\boldsymbol{B}} = 2\,(\boldsymbol{B}\boldsymbol{D}\boldsymbol{B}) - (\boldsymbol{B}\boldsymbol{A}^c) - (\boldsymbol{B}\boldsymbol{A}^c)^\dagger \\ \boldsymbol{B}\dot{\boldsymbol{X}}^0 = -\boldsymbol{B}\boldsymbol{A}^c\,\boldsymbol{X}^0 \\ \dot{C}(t) = -\mathrm{Tr}(\boldsymbol{D}\boldsymbol{B} - \boldsymbol{A}^c). \end{cases} \tag{B5}$$

The first equation implies for $\boldsymbol{B}^{-1}$:

$$\frac{d}{dt}\boldsymbol{B}^{-1} = 2\boldsymbol{D} - \boldsymbol{A}\boldsymbol{B}^{-1} - \boldsymbol{B}^{-1}\boldsymbol{A}^\dagger, \tag{B6}$$

which can be integrated to give:

$$\boldsymbol{B}^{-1} = 2\int_0^t \boldsymbol{U}(t)\boldsymbol{U}^{-1}(t')\boldsymbol{D}\boldsymbol{U}^{\dagger^{-1}}(t')\boldsymbol{U}^\dagger(t)dt' + \boldsymbol{U}(t)\sigma_0\boldsymbol{U}^\dagger(t). \tag{B7}$$

Multiplying the second equation by B^{-1} on the left, one gets

$$\dot{X}_l^0 = -A_{lm}^c\,X_m^0, \tag{B8}$$

which means that $\boldsymbol{X}^0$ follows the noiseless evolution. Equation (36) tells us that

$$X_i^0(t) = U_{ij}^c(t)\,X_j^0(0) \tag{B9}$$

are solutions of (B8).

From the normalization of P, we get:

$$\sqrt{\frac{\det \boldsymbol{B}(t)}{(2\pi)^N}} = e^{C(t)}, \tag{B10}$$

which satisfies the third equation of (B5). Starting with $P(\boldsymbol{X}, 0) = \delta(\boldsymbol{X} - \boldsymbol{Y})$, i.e. $\boldsymbol{X}^0(0) = \boldsymbol{Y}$ and $B_{ij}(0) = \lim_{\Delta\to\infty}\Delta\delta_{ij}$, the density is:

$$P_Y(\boldsymbol{X}, t) = \sqrt{\frac{\det \boldsymbol{B}(t)}{(2\pi)^N}}e^{-\frac{B_{ij}}{2}(X_i - U_{ik}^c Y_k)(X_j - U_{jl}^c Y_l)}. \tag{B11}$$

The trace now reads

$$\int P_Y(\boldsymbol{Y}, t)d\boldsymbol{Y} = \sqrt{\frac{\det \boldsymbol{B}}{(2\pi)^N}}\sqrt{\frac{(2\pi)^N}{\det\left(1 - U^c(t)\right)^\dagger \det \boldsymbol{B} \det\left(1 - U^c(t)\right)}}, \tag{B12}$$

that is:

$$\int P_Y(\boldsymbol{Y}, t)d\boldsymbol{Y} = \frac{1}{|\det\left(1 - U^c(t)\right)|}. \tag{B13}$$

Therefore, the bosonic contribution of a classical periodic orbit is $\frac{1}{|\det(1-U^c)|}$.

The fermionic counterpart to this contribution is obtained by taking

$$\sum_p \lambda^p \, \text{Tr} \left(\mathcal{T} e^{-\int A_{ij}^c c_i^\dagger c_j} \right) \Big|_{\text{p ferm.}} = \sum_p \lambda^p \sum_{i_1,\dots,i_p} \langle -|c_{i_1} \dots c_{i_p} \mathcal{T} \, e^{-\int A_{ij}^c c_i^\dagger c_j} c_{i_p}^\dagger \dots c_{i_1}^\dagger |-\rangle,$$

(B14)

where the time-order is defined along the noiseless trajectory. Let us first calculate the terms $\langle -|c_{i_1} \dots c_{i_p} \mathcal{T} \, e^{-\int A_{ij}^c c_i^\dagger c_j} c_{i_p}^\dagger \dots c_{i_1}^\dagger |-\rangle$. Using the fact that:

$$\left(\mathcal{T} e^{-\int_0^t A_{ij}^c c_i^\dagger c_j} \right) c_{i_l}^\dagger \left(\mathcal{T} e^{\int_0^t A_{ij}^c c_i^\dagger c_j} \right) = U_{i_k i_l}^c(t) c_{i_k}^\dagger,$$

(B15)

which can easily be seen by differentiating right and left with respect to t, and denoting $O = \mathcal{T} e^{-\int A_{ij}^c c_i^\dagger c_j}$, we get:

$$\langle -|c_{i_1} \dots c_{i_p} O c_{i_p}^\dagger \dots c_{i_1}^\dagger |-\rangle = \langle -|c_{i_1}, \dots c_{i_p} O c_{i_p}^\dagger O^{-1} \, O c_{i_{p-1}}^\dagger O^{-1} \dots O c_{i_1}^\dagger O^{-1} |-\rangle$$

$$= \langle -|c_{i_1}, \dots c_{i_p} \sum_{j_p} U_{j_p i_p}^c c_{j_p}^\dagger \sum_{j_{p-1}} U_{j_{p-1} i_{p-1}}^c c_{j_{p-1}}^\dagger \dots \sum_{j_1} U_{j_1 i_1}^c c_{j_1}^\dagger |-\rangle$$

$$= \sum_{j_1 \dots j_p} \prod_{k=1}^p U_{j_k i_k}^c \langle -|c_{i_1}, \dots c_{i_p} c_{j_p}^\dagger, \dots c_{j_1}^\dagger |-\rangle.$$

(B16)

For a bracket to be non-zero, $j_1, \cdots, j_p$ must be a permutation of $i_1, \cdots, i_p$. The scalar product is then the sign of the permutation, and one has:

$$\langle -|c_{i_1}, \dots c_{i_p} O c_{i_p}^\dagger, \dots c_{i_1}^\dagger |-\rangle = \det_p U_{i_1,\dots,i_p}^c,$$

(B17)

where $\det_p U_{i_1,\dots,i_p}^c$ is the minor of order p of $U^c(t)$ associated with the directions $i_1, \dots, i_p$. We can now compute the generating function of the fermionic orbit's contribution:

$$\sum_p \lambda^p \text{Tr} \, \mathcal{T} e^{-\int_0^t A_{ij}^c c_i^\dagger c_j} \Big|_{\text{p fermions}} = \sum_p \lambda^p \sum_{i_1,\dots,i_p} \det_p U_{i_1,\dots,i_p}^c$$

$$= \det \left(1 + \lambda U^c(t) \right).$$

(B18)

Putting all together, the generating function of the contribution of a classical periodic orbit 'c' is:

$$T^c(\lambda, t) = \frac{\det \left(1 + \lambda U^c(t) \right)}{|\det \left(1 - U^c(t) \right)|},$$

(B19)

and we hence have:

$$T(\lambda, t) = \sum_{\substack{\text{noiseless} \\ \text{orbits c}}} \frac{\det \left(1 + \lambda U^c(t) \right)}{|\det \left(1 - U^c(t) \right)|}.$$

(B20)

APPENDIX C

Let us consider a single saddle point (we drop the label 'c'), which we assume is at the origin. We develop V to second order in q_i, and may assume further that $\frac{\partial^2 V}{\partial q_i \partial q_j}(0)$ is diagonalized. We can hence treat each mode separately, so for ease of notation we drop the sub-indices i, j. We wish to construct for each mode of each saddle point, an eigenvector that is zero to this order:

$$H^c |\psi_h\rangle = 0, \tag{C1}$$

that is, for some λ:

$$\begin{cases} \left(-\gamma T \frac{\partial^2}{\partial p^2} - \frac{\gamma}{2} + \frac{\gamma}{4T} p^2 - V'' q \frac{\partial}{\partial p} + p \frac{\partial}{\partial q}\right) |\psi_b^{hR}\rangle = \lambda |\psi_b^{hR}\rangle \\ \left(V'' b^\dagger a + \gamma b^\dagger b - a^\dagger b\right) |\psi_f^{hR}\rangle = -\lambda |\psi_f^{hR}\rangle. \end{cases} \tag{C2}$$

Let us first have a look at the fermionic part. In the basis $|-\rangle, |a^\dagger\rangle, |b^\dagger\rangle, |a^\dagger b^\dagger\rangle$, the fermionic part of (C2) reads:

$$H_{\text{ferm.}} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & V'' & \gamma & 0 \\ 0 & 0 & 0 & \gamma \end{pmatrix}. \tag{C3}$$

The spectrum and the corresponding eigenvectors are easily obtained:

$$\lambda = 0 \leftrightarrow |\psi_f^{hR}\rangle = |-\rangle$$

$$\lambda = \frac{\gamma}{2} \pm \frac{1}{2}\sqrt{\gamma^2 - 4V''} \leftrightarrow |\psi_f^{hR}\rangle = -\gamma \pm \sqrt{\gamma^2 - 4V''}|a^\dagger\rangle + 2V''|b^\dagger\rangle \tag{C4}$$

$$\lambda = \gamma \leftrightarrow |\psi_f^{hR}\rangle = |a^\dagger b^\dagger\rangle.$$

Regarding the bosonic part of (C2), the Gaussian form of the eigenvector allows us to compute the l.h.s:

$$H_{\text{bos.}} |\psi_b^{hR}\rangle = \left(\left(B_{pp} - \frac{1}{2}\right)\gamma + \left(\frac{\gamma}{4} - \gamma B_{pp}^2 - B_{pq}\right)\frac{p^2}{T} + \left(V'' B_{pq} - \gamma B_{pq}^2\right)\frac{q^2}{T}\right.$$

$$\left. + \left(-2\gamma B_{pq} B_{pp} + V'' B_{pp} + B_{qq}\right)\frac{pq}{T}\right) |\psi_b^{hR}\rangle. \tag{C5}$$

The prefactor of the quadratic terms must be equal to zero. On the other hand, the Gaussian must be well normalized, i.e. the eigenvectors of B must be positive. After a tedious but straightforward calculation, two solutions are possible, depending on the sign of V'':

- if $V'' > 0$, then $B_{pp} = \frac{1}{2}$, $B_{pq} = 0$ and $B_{qq} = \frac{V''}{2}$. This corresponds to an eigenvalue 0 for the bosonic part, and the corresponding fermionic part is thus the vacuum:

$$|\psi^{hR}_{V''>0}\rangle = e^{-\frac{1}{4T}(p^2 + V''q^2)} \otimes |-\rangle; \qquad (C6)$$

- if $V'' < 0$, then $B_{pp} = \frac{\sqrt{\gamma^2 - 4V''}}{2\gamma}$, $B_{pq} = \frac{V''}{\gamma}$ and $B_{qq} = -V'' \frac{\sqrt{\gamma^2 - 4V''}}{2\gamma}$. This corresponds to an eigenvalue $-\frac{\gamma}{2} + \frac{\sqrt{\gamma^2 - 4V''}}{2}$ for the bosonic part, which is compensated by the corresponding fermionic part $(-\gamma - \sqrt{\gamma^2 - 4V''})|a^\dagger\rangle + 2V''|b^\dagger\rangle$:

$$|\psi^{hR}_{V''<0}\rangle = e^{-\frac{\sqrt{\gamma^2-4V''}}{4\gamma T}(p^2 - V''q^2) - \frac{1}{2\gamma T}V''pq}$$
$$\otimes ((-\gamma - \sqrt{\gamma^2 - 4V''})|a^\dagger\rangle + 2V''|b^\dagger\rangle). \qquad (C7)$$

The same development for $H^\dagger$ leads to:

- if $V'' > 0$, then $B_{pp} = \frac{1}{2}$, $B_{pq} = 0$ and $B_{qq} = \frac{V''}{2}$. This corresponds to an eigenvalue 0 for the bosonic part, and the corresponding fermionic part is thus the vacuum:

$$|\psi^{hL}_{V''>0}\rangle = e^{-\frac{1}{4T}(p^2 + V''q^2)} \otimes |-\rangle; \qquad (C8)$$

- if $V'' < 0$, then $B_{pp} = \frac{\sqrt{\gamma^2 - 4V''}}{2\gamma}$, $B_{pq} = -\frac{V''}{\gamma}$ and $B_{qq} = -V'' \frac{\sqrt{\gamma^2 - 4V''}}{2\gamma}$. This corresponds to an eigenvalue $-\frac{\gamma}{2} + \frac{\sqrt{\gamma^2 - 4V''}}{2}$, for the bosonic part, which is compensated by the corresponding fermionic part $(\gamma + \sqrt{\gamma^2 - 4V''})|a^\dagger\rangle + 2|b^\dagger\rangle$:

$$|\psi^{hL}_{V''<0}\rangle = e^{-\frac{\sqrt{\gamma^2-4V''}}{4\gamma T}(p^2 - V''q^2) + \frac{1}{2\gamma T}V''pq} \otimes ((\gamma + \sqrt{\gamma^2 - 4V''})|a^\dagger\rangle + 2|b^\dagger\rangle). \qquad (C9)$$

The structure of the spectrum can be directly seen in the eigenvectors: a stable direction corresponds to the fermionic vacuum while an unstable direction corresponds to a one-fermion state. We have also shown that both the right and left eigenvectors with zero eigenvalue are Gaussians to this order in the new basis.

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